



Full wwPDB EM Validation Report ⓘ

Jul 7, 2021 – 11:23 am BST

PDB ID : 7OI0
EMDB ID : EMD-12916
Title : E.coli delta rbfA pre-30S ribosomal subunit class D
Authors : Maksimova, E.; Korepanov, A.; Baymukhametov, T.; Kravchenko, O.; Stoboushkina, E.
Deposited on : 2021-05-11
Resolution : 2.76 Å(reported)
Based on initial model : 4V4Q

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

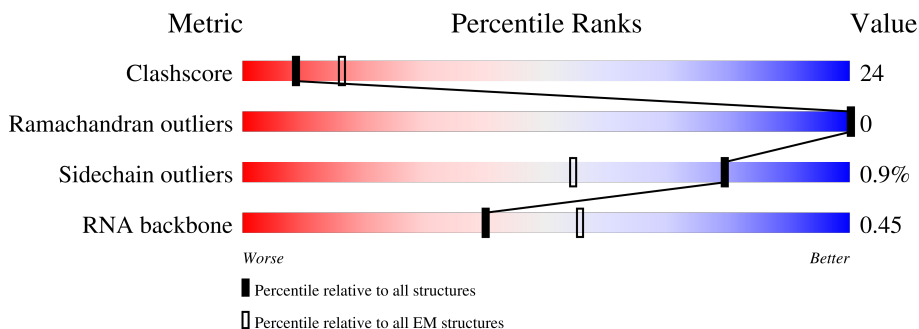
EMDB validation analysis : 0.0.0.dev84
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.22

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.76 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




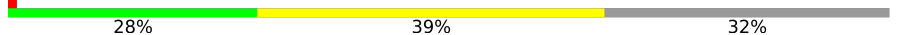


| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |
| RNA backbone | 4643 | 859 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | D | 205 | 59% (green), 40% (yellow), . (grey) |
| 2 | F | 135 | 10% (red), 33% (green), 41% (yellow), 26% (grey) |
| 3 | H | 129 | 61% (green), 39% (yellow) |
| 4 | K | 128 | 49% (red), 39% (green), 34% (yellow), 26% (grey), . (grey) |
| 5 | L | 123 | 59% (green), 41% (yellow), . (grey) |
| 6 | O | 89 | 48% (green), 51% (yellow), . (grey) |
| 7 | P | 82 | 63% (green), 35% (yellow), . (grey) |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 8 | Q | 83 |  57% 40% |
| 9 | R | 74 |  28% 39% 32% |
| 10 | T | 86 |  69% 30% |
| 11 | A | 1542 |  13% 32% 16% 38% |

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 29255 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 1 | D | 205 | 1643 | 1026 | 315 | 298 | 4 | 0 | 0 |

- Molecule 2 is a protein called 30S ribosomal protein S6, fully modified isoform.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 2 | F | 100 | 817 | 515 | 148 | 148 | 6 | 0 | 0 |

- Molecule 3 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 3 | H | 129 | 979 | 616 | 173 | 184 | 6 | 0 | 0 |

- Molecule 4 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 4 | K | 95 | 702 | 433 | 137 | 130 | 2 | 0 | 0 |

- Molecule 5 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 5 | L | 123 | 955 | 590 | 196 | 165 | 4 | 0 | 0 |

- Molecule 6 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 6 | O | 88 | 716 | 440 | 146 | 129 | 1 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|----------------|
| O | 79 | ARG | GLN | conflict | UNP A0A4S5B232 |

- Molecule 7 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 7 | P | 82 | 649 | 406 | 128 | 114 | 1 | 0 | 0 |

- Molecule 8 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 8 | Q | 80 | 648 | 411 | 121 | 113 | 3 | 0 | 0 |

- Molecule 9 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| | | | Total | C | N | O | | |
| 9 | R | 50 | 407 | 259 | 76 | 72 | 0 | 0 |

- Molecule 10 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 10 | T | 85 | 665 | 411 | 137 | 114 | 3 | 0 | 0 |

- Molecule 11 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|-----|---------|-------|
| | | | Total | C | N | O | P | | |
| 11 | A | 963 | 20700 | 9228 | 3823 | 6686 | 963 | 0 | 0 |

- Molecule 12 is water.

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 12 | D | 6 | Total | O | 0 |
| | | | 6 | 6 | |
| 12 | L | 4 | Total | O | 0 |
| | | | 4 | 4 | |
| 12 | P | 18 | Total | O | 0 |
| | | | 18 | 18 | |

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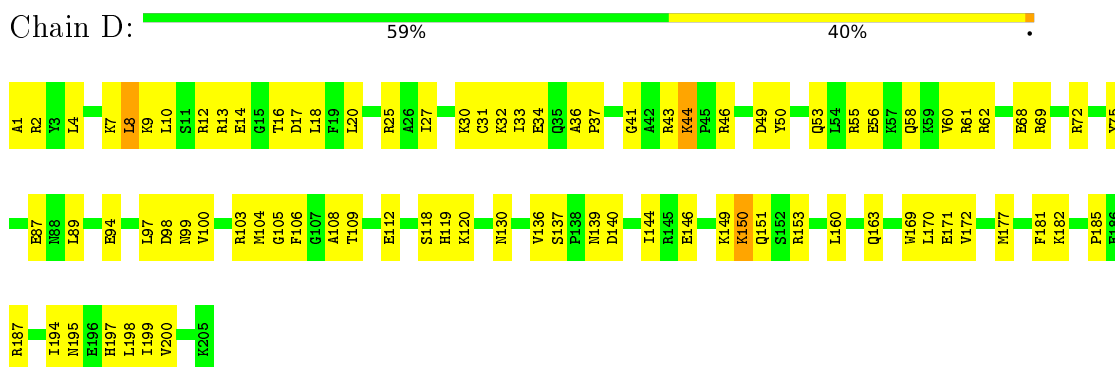
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| Mol | Chain | Residues | Atoms | | AltConf |
|------------|--------------|-----------------|--------------|----------|----------------|
| 12 | Q | 3 | Total 3 | O 3 | 0 |
| 12 | T | 6 | Total 6 | O 6 | 0 |
| 12 | A | 337 | Total 337 | O 337 | 0 |

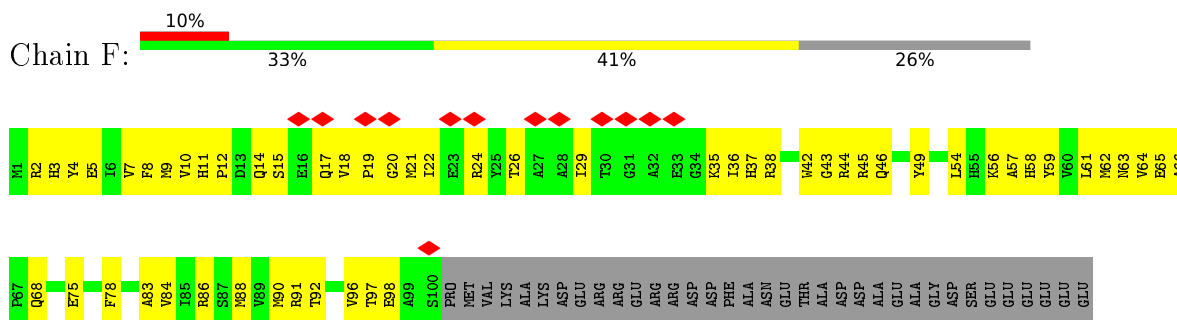
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

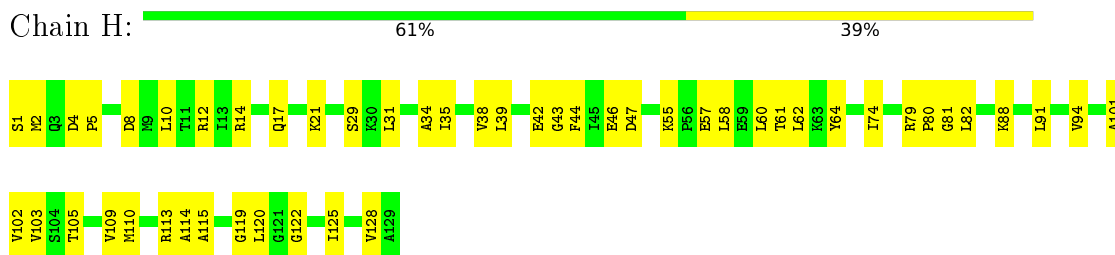
- Molecule 1: 30S ribosomal protein S4



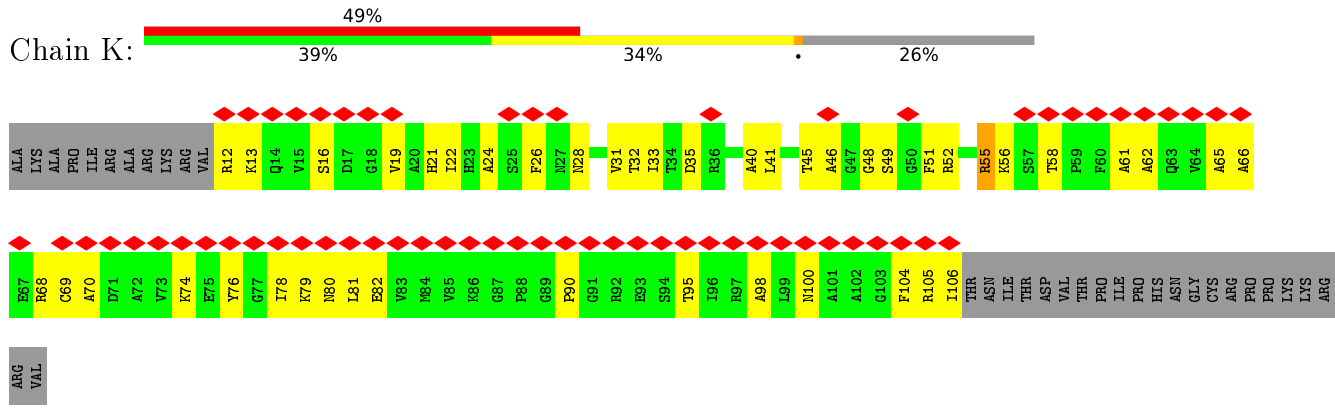
- Molecule 2: 30S ribosomal protein S6, fully modified isoform



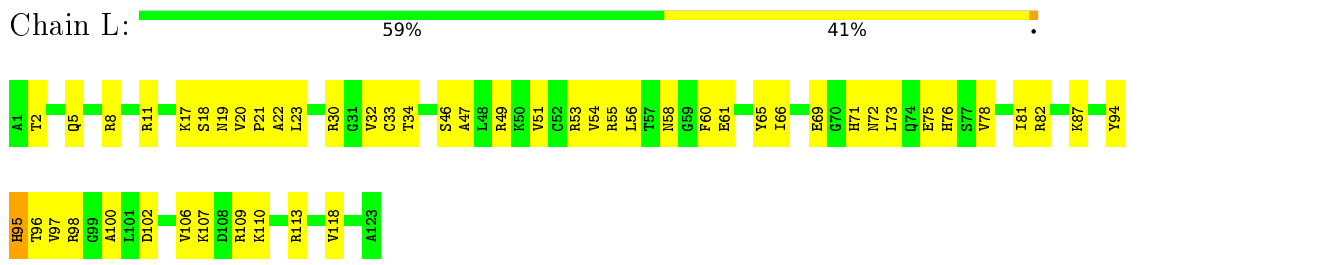
- Molecule 3: 30S ribosomal protein S8



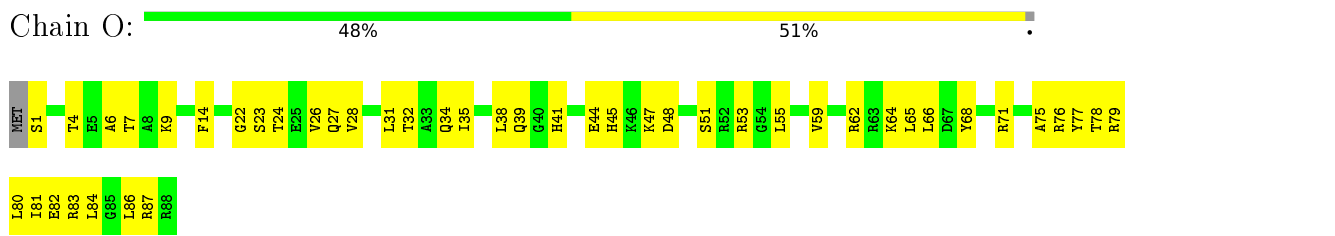
- Molecule 4: 30S ribosomal protein S11



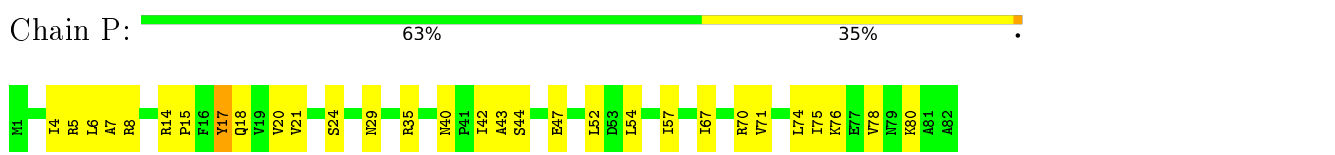
• Molecule 5: 30S ribosomal protein S12



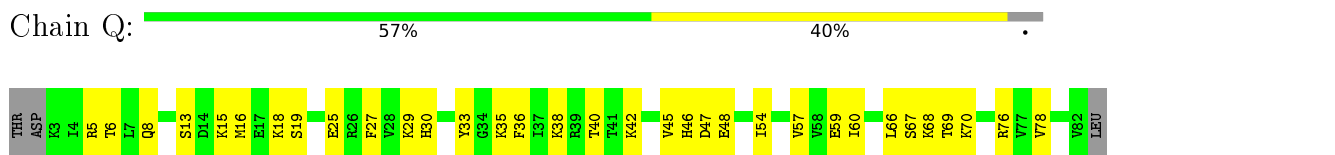
• Molecule 6: 30S ribosomal protein S15



• Molecule 7: 30S ribosomal protein S16

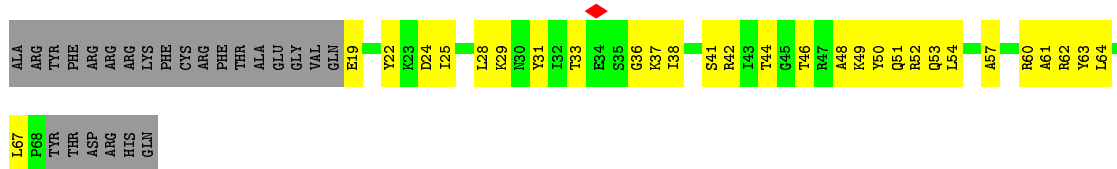


• Molecule 8: 30S ribosomal protein S17



• Molecule 9: 30S ribosomal protein S18

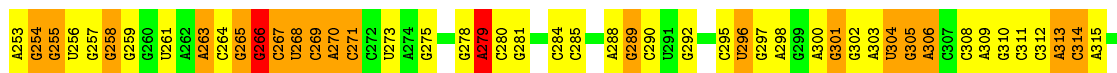
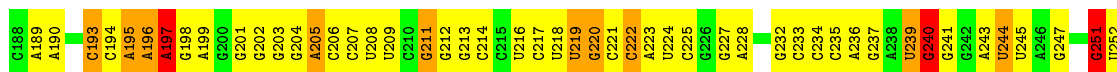
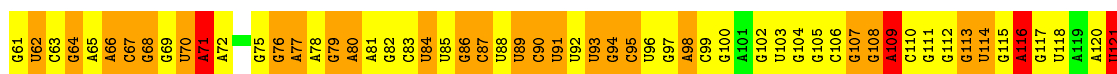




• Molecule 10: 30S ribosomal protein S20



• Molecule 11: 16S rRNA



4 Experimental information

| Property | Value | Source |
|--------------------------------------|-------------------------|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 106319 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING ONLY | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 2.5 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | FEI FALCON II (4k x 4k) | Depositor |
| Maximum map value | 5.611 | Depositor |
| Minimum map value | -2.640 | Depositor |
| Average map value | 0.007 | Depositor |
| Map value standard deviation | 0.083 | Depositor |
| Recommended contour level | 0.218 | Depositor |
| Map size (\AA) | 378.4, 378.4, 378.4 | wwPDB |
| Map dimensions | 440, 440, 440 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 0.86, 0.86, 0.86 | Depositor |

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | D | 0.62 | 0/1665 | 0.67 | 0/2227 |
| 2 | F | 0.29 | 0/835 | 0.48 | 0/1128 |
| 3 | H | 0.47 | 0/989 | 0.61 | 0/1326 |
| 4 | K | 0.26 | 0/713 | 0.46 | 0/960 |
| 5 | L | 0.68 | 0/969 | 0.77 | 0/1300 |
| 6 | O | 0.41 | 0/724 | 0.53 | 0/966 |
| 7 | P | 1.03 | 2/659 (0.3%) | 0.79 | 0/884 |
| 8 | Q | 0.80 | 0/657 | 0.68 | 0/881 |
| 9 | R | 0.25 | 0/412 | 0.46 | 0/553 |
| 10 | T | 0.66 | 0/671 | 0.69 | 0/888 |
| 11 | A | 1.71 | 381/23184 (1.6%) | 1.20 | 132/36171 (0.4%) |
| All | All | 1.50 | 383/31478 (1.2%) | 1.10 | 132/47284 (0.3%) |

All (383) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 11 | A | 452 | A | N9-C4 | -10.64 | 1.31 | 1.37 |
| 11 | A | 353 | A | N9-C4 | -10.25 | 1.31 | 1.37 |
| 11 | A | 355 | C | N3-C4 | -8.73 | 1.27 | 1.33 |
| 11 | A | 113 | G | C6-N1 | -8.63 | 1.33 | 1.39 |
| 11 | A | 394 | G | C5-C4 | -7.84 | 1.32 | 1.38 |
| 11 | A | 102 | G | C6-N1 | -7.76 | 1.34 | 1.39 |
| 11 | A | 322 | C | N3-C4 | -7.61 | 1.28 | 1.33 |
| 11 | A | 329 | A | N7-C5 | -7.57 | 1.34 | 1.39 |
| 11 | A | 152 | A | N9-C4 | -7.56 | 1.33 | 1.37 |
| 11 | A | 377 | G | C2-N3 | -7.49 | 1.26 | 1.32 |
| 11 | A | 354 | G | C6-N1 | -7.49 | 1.34 | 1.39 |
| 11 | A | 387 | U | C2-N3 | -7.49 | 1.32 | 1.37 |
| 11 | A | 391 | G | C6-N1 | -7.45 | 1.34 | 1.39 |
| 11 | A | 378 | G | C8-N7 | -7.33 | 1.26 | 1.30 |
| 11 | A | 324 | G | C5-C4 | -7.24 | 1.33 | 1.38 |
| 11 | A | 393 | A | C5-C4 | -7.18 | 1.33 | 1.38 |
| 11 | A | 449 | G | C5-C4 | -7.15 | 1.33 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 11 | A | 401 | C | N3-C4 | -7.12 | 1.28 | 1.33 |
| 11 | A | 450 | G | C6-N1 | -7.11 | 1.34 | 1.39 |
| 11 | A | 106 | C | N1-C6 | -7.10 | 1.32 | 1.37 |
| 11 | A | 61 | G | C6-N1 | -7.09 | 1.34 | 1.39 |
| 11 | A | 450 | G | C5-C4 | -7.04 | 1.33 | 1.38 |
| 11 | A | 107 | G | N9-C8 | -7.03 | 1.32 | 1.37 |
| 11 | A | 391 | G | C8-N7 | -7.01 | 1.26 | 1.30 |
| 11 | A | 310 | G | C6-N1 | -6.99 | 1.34 | 1.39 |
| 11 | A | 113 | G | C5-C4 | -6.97 | 1.33 | 1.38 |
| 11 | A | 618 | C | N3-C4 | -6.97 | 1.29 | 1.33 |
| 11 | A | 45 | G | C5-C4 | -6.96 | 1.33 | 1.38 |
| 11 | A | 354 | G | C8-N7 | -6.95 | 1.26 | 1.30 |
| 11 | A | 109 | A | C8-N7 | -6.94 | 1.26 | 1.31 |
| 11 | A | 378 | G | C6-N1 | -6.94 | 1.34 | 1.39 |
| 11 | A | 108 | G | C5-C6 | -6.92 | 1.35 | 1.42 |
| 11 | A | 117 | G | C6-N1 | -6.91 | 1.34 | 1.39 |
| 11 | A | 311 | C | N3-C4 | -6.87 | 1.29 | 1.33 |
| 11 | A | 379 | C | N3-C4 | -6.87 | 1.29 | 1.33 |
| 11 | A | 257 | G | C6-N1 | -6.84 | 1.34 | 1.39 |
| 11 | A | 390 | U | C2-N3 | -6.82 | 1.32 | 1.37 |
| 11 | A | 42 | G | C5-C4 | -6.81 | 1.33 | 1.38 |
| 11 | A | 384 | G | N1-C2 | -6.79 | 1.32 | 1.37 |
| 11 | A | 332 | G | C8-N7 | -6.76 | 1.26 | 1.30 |
| 11 | A | 181 | A | C5-C4 | -6.74 | 1.34 | 1.38 |
| 11 | A | 107 | G | C8-N7 | -6.71 | 1.26 | 1.30 |
| 11 | A | 357 | G | C6-N1 | -6.71 | 1.34 | 1.39 |
| 11 | A | 59 | A | N9-C4 | -6.71 | 1.33 | 1.37 |
| 11 | A | 393 | A | N7-C5 | -6.70 | 1.35 | 1.39 |
| 11 | A | 35 | G | C8-N7 | -6.70 | 1.26 | 1.30 |
| 11 | A | 112 | G | C5-C4 | -6.70 | 1.33 | 1.38 |
| 11 | A | 402 | G | C6-N1 | -6.67 | 1.34 | 1.39 |
| 11 | A | 113 | G | C8-N7 | -6.66 | 1.26 | 1.30 |
| 11 | A | 391 | G | N7-C5 | -6.63 | 1.35 | 1.39 |
| 11 | A | 449 | G | C2-N3 | -6.60 | 1.27 | 1.32 |
| 11 | A | 127 | G | C6-N1 | -6.57 | 1.34 | 1.39 |
| 11 | A | 46 | G | C6-N1 | -6.57 | 1.34 | 1.39 |
| 11 | A | 292 | G | C8-N7 | -6.57 | 1.27 | 1.30 |
| 11 | A | 54 | C | N1-C6 | -6.56 | 1.33 | 1.37 |
| 11 | A | 66 | A | C6-N1 | -6.55 | 1.30 | 1.35 |
| 11 | A | 369 | G | C6-N1 | -6.54 | 1.34 | 1.39 |
| 11 | A | 112 | G | C8-N7 | -6.50 | 1.27 | 1.30 |
| 11 | A | 117 | G | C5-C4 | -6.50 | 1.33 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 11 | A | 403 | C | C2-N3 | -6.50 | 1.30 | 1.35 |
| 11 | A | 133 | U | C2-N3 | -6.49 | 1.33 | 1.37 |
| 11 | A | 392 | C | N3-C4 | -6.49 | 1.29 | 1.33 |
| 11 | A | 182 | A | N9-C4 | -6.47 | 1.33 | 1.37 |
| 11 | A | 354 | G | C2-N3 | -6.44 | 1.27 | 1.32 |
| 11 | A | 393 | A | N9-C8 | -6.37 | 1.32 | 1.37 |
| 11 | A | 43 | C | N3-C4 | -6.35 | 1.29 | 1.33 |
| 11 | A | 109 | A | N7-C5 | -6.35 | 1.35 | 1.39 |
| 11 | A | 546 | A | N9-C4 | -6.35 | 1.34 | 1.37 |
| 11 | A | 353 | A | N3-C4 | -6.34 | 1.31 | 1.34 |
| 11 | A | 37 | U | C2-N3 | -6.32 | 1.33 | 1.37 |
| 11 | A | 625 | U | C2-N3 | -6.30 | 1.33 | 1.37 |
| 11 | A | 255 | G | C6-N1 | -6.28 | 1.35 | 1.39 |
| 11 | A | 370 | C | N3-C4 | -6.24 | 1.29 | 1.33 |
| 11 | A | 488 | C | N1-C6 | -6.24 | 1.33 | 1.37 |
| 11 | A | 38 | G | C5-C4 | -6.23 | 1.33 | 1.38 |
| 11 | A | 384 | G | C8-N7 | -6.22 | 1.27 | 1.30 |
| 11 | A | 624 | C | N3-C4 | -6.22 | 1.29 | 1.33 |
| 11 | A | 292 | G | C5-C4 | -6.21 | 1.33 | 1.38 |
| 11 | A | 45 | G | C6-N1 | -6.21 | 1.35 | 1.39 |
| 11 | A | 108 | G | N9-C4 | -6.19 | 1.32 | 1.38 |
| 11 | A | 609 | A | N9-C4 | -6.14 | 1.34 | 1.37 |
| 11 | A | 322 | C | N1-C6 | -6.13 | 1.33 | 1.37 |
| 11 | A | 326 | G | C5-C4 | -6.12 | 1.34 | 1.38 |
| 11 | A | 371 | A | C2-N3 | -6.12 | 1.28 | 1.33 |
| 11 | A | 107 | G | C5-C4 | -6.12 | 1.34 | 1.38 |
| 11 | A | 61 | G | C2-N3 | -6.11 | 1.27 | 1.32 |
| 11 | A | 354 | G | C5-C6 | -6.11 | 1.36 | 1.42 |
| 11 | A | 112 | G | C6-N1 | -6.11 | 1.35 | 1.39 |
| 11 | A | 371 | A | C5-C4 | -6.11 | 1.34 | 1.38 |
| 11 | A | 108 | G | N7-C5 | -6.10 | 1.35 | 1.39 |
| 11 | A | 548 | G | C6-N1 | -6.10 | 1.35 | 1.39 |
| 11 | A | 323 | U | C2-N3 | -6.10 | 1.33 | 1.37 |
| 11 | A | 378 | G | C2-N3 | -6.09 | 1.27 | 1.32 |
| 11 | A | 362 | G | C5-C4 | -6.09 | 1.34 | 1.38 |
| 11 | A | 240 | G | C6-N1 | -6.09 | 1.35 | 1.39 |
| 11 | A | 263 | A | N9-C4 | -6.07 | 1.34 | 1.37 |
| 11 | A | 377 | G | C5-C4 | -6.07 | 1.34 | 1.38 |
| 11 | A | 389 | A | C6-N6 | -6.06 | 1.29 | 1.33 |
| 11 | A | 57 | G | C6-N1 | -6.05 | 1.35 | 1.39 |
| 11 | A | 54 | C | C2-N3 | -6.05 | 1.30 | 1.35 |
| 11 | A | 312 | C | C4-C5 | -6.05 | 1.38 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 11 | A | 181 | A | N9-C4 | -6.04 | 1.34 | 1.37 |
| 11 | A | 393 | A | N9-C4 | -6.04 | 1.34 | 1.37 |
| 11 | A | 449 | G | C6-N1 | -6.03 | 1.35 | 1.39 |
| 11 | A | 378 | G | C5-C4 | -6.03 | 1.34 | 1.38 |
| 11 | A | 232 | G | C2-N3 | -6.01 | 1.27 | 1.32 |
| 11 | A | 113 | G | N1-C2 | -6.01 | 1.32 | 1.37 |
| 11 | A | 42 | G | C6-N1 | -6.01 | 1.35 | 1.39 |
| 11 | A | 331 | G | C8-N7 | -6.00 | 1.27 | 1.30 |
| 11 | A | 222 | C | N1-C6 | -6.00 | 1.33 | 1.37 |
| 11 | A | 392 | C | C2-N3 | -6.00 | 1.30 | 1.35 |
| 11 | A | 233 | C | N3-C4 | -6.00 | 1.29 | 1.33 |
| 11 | A | 388 | G | C6-N1 | -5.99 | 1.35 | 1.39 |
| 11 | A | 326 | G | C8-N7 | -5.99 | 1.27 | 1.30 |
| 11 | A | 356 | A | C5-C4 | -5.99 | 1.34 | 1.38 |
| 11 | A | 290 | C | N3-C4 | -5.98 | 1.29 | 1.33 |
| 11 | A | 292 | G | C6-N1 | -5.98 | 1.35 | 1.39 |
| 11 | A | 42 | G | C2-N3 | -5.98 | 1.27 | 1.32 |
| 11 | A | 402 | G | C5-C4 | -5.98 | 1.34 | 1.38 |
| 11 | A | 404 | G | C5-C4 | -5.97 | 1.34 | 1.38 |
| 11 | A | 41 | G | C2-N3 | -5.97 | 1.27 | 1.32 |
| 11 | A | 263 | A | C5-C4 | -5.96 | 1.34 | 1.38 |
| 11 | A | 41 | G | C6-N1 | -5.95 | 1.35 | 1.39 |
| 11 | A | 482 | A | N7-C5 | -5.95 | 1.35 | 1.39 |
| 11 | A | 377 | G | C6-N1 | -5.94 | 1.35 | 1.39 |
| 11 | A | 391 | G | C2-N3 | -5.94 | 1.27 | 1.32 |
| 11 | A | 324 | G | N1-C2 | -5.93 | 1.33 | 1.37 |
| 11 | A | 289 | G | C8-N7 | -5.93 | 1.27 | 1.30 |
| 11 | A | 135 | C | N3-C4 | -5.92 | 1.29 | 1.33 |
| 11 | A | 360 | G | C2-N3 | -5.92 | 1.28 | 1.32 |
| 11 | A | 271 | C | C2-N3 | -5.91 | 1.31 | 1.35 |
| 11 | A | 308 | C | N3-C4 | -5.91 | 1.29 | 1.33 |
| 11 | A | 354 | G | N7-C5 | -5.90 | 1.35 | 1.39 |
| 11 | A | 325 | A | C5-C4 | -5.90 | 1.34 | 1.38 |
| 11 | A | 305 | G | C8-N7 | -5.89 | 1.27 | 1.30 |
| 11 | A | 181 | A | C8-N7 | -5.88 | 1.27 | 1.31 |
| 11 | A | 124 | C | N3-C4 | -5.86 | 1.29 | 1.33 |
| 11 | A | 330 | C | N3-C4 | -5.86 | 1.29 | 1.33 |
| 11 | A | 384 | G | C6-N1 | -5.84 | 1.35 | 1.39 |
| 11 | A | 69 | G | C8-N7 | -5.84 | 1.27 | 1.30 |
| 11 | A | 193 | C | N1-C6 | -5.84 | 1.33 | 1.37 |
| 11 | A | 621 | A | N7-C5 | -5.84 | 1.35 | 1.39 |
| 11 | A | 59 | A | C8-N7 | -5.83 | 1.27 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 11 | A | 360 | G | C5-C4 | -5.83 | 1.34 | 1.38 |
| 11 | A | 402 | G | N1-C2 | -5.83 | 1.33 | 1.37 |
| 11 | A | 495 | A | N7-C5 | -5.83 | 1.35 | 1.39 |
| 11 | A | 109 | A | N9-C8 | -5.81 | 1.33 | 1.37 |
| 11 | A | 358 | U | N3-C4 | -5.81 | 1.33 | 1.38 |
| 11 | A | 117 | G | N1-C2 | -5.81 | 1.33 | 1.37 |
| 11 | A | 147 | G | C6-N1 | -5.80 | 1.35 | 1.39 |
| 11 | A | 369 | G | C8-N7 | -5.80 | 1.27 | 1.30 |
| 11 | A | 128 | G | C8-N7 | -5.79 | 1.27 | 1.30 |
| 11 | A | 481 | G | C6-N1 | -5.79 | 1.35 | 1.39 |
| 11 | A | 371 | A | C6-N1 | -5.78 | 1.31 | 1.35 |
| 11 | A | 372 | C | N3-C4 | -5.77 | 1.29 | 1.33 |
| 11 | A | 223 | A | N9-C4 | -5.77 | 1.34 | 1.37 |
| 11 | A | 46 | G | C5-C4 | -5.76 | 1.34 | 1.38 |
| 11 | A | 501 | C | N3-C4 | -5.76 | 1.29 | 1.33 |
| 11 | A | 392 | C | N1-C6 | -5.74 | 1.33 | 1.37 |
| 11 | A | 451 | A | N9-C4 | -5.74 | 1.34 | 1.37 |
| 11 | A | 503 | C | N3-C4 | -5.74 | 1.29 | 1.33 |
| 11 | A | 251 | G | C5-C4 | 5.74 | 1.42 | 1.38 |
| 11 | A | 377 | G | C8-N7 | -5.74 | 1.27 | 1.30 |
| 11 | A | 134 | G | C8-N7 | -5.73 | 1.27 | 1.30 |
| 11 | A | 241 | G | C5-C4 | -5.72 | 1.34 | 1.38 |
| 11 | A | 175 | C | N3-C4 | -5.71 | 1.29 | 1.33 |
| 11 | A | 332 | G | C5-C4 | -5.71 | 1.34 | 1.38 |
| 11 | A | 617 | G | C5-C4 | -5.71 | 1.34 | 1.38 |
| 11 | A | 240 | G | C2-N3 | -5.70 | 1.28 | 1.32 |
| 11 | A | 395 | C | N3-C4 | -5.70 | 1.29 | 1.33 |
| 7 | P | 20 | VAL | CB-CG2 | -5.69 | 1.40 | 1.52 |
| 11 | A | 268 | U | C2-N3 | -5.69 | 1.33 | 1.37 |
| 11 | A | 354 | G | C5-C4 | -5.69 | 1.34 | 1.38 |
| 11 | A | 361 | G | C2-N3 | -5.69 | 1.28 | 1.32 |
| 11 | A | 501 | C | N1-C6 | -5.68 | 1.33 | 1.37 |
| 11 | A | 41 | G | C5-C4 | -5.68 | 1.34 | 1.38 |
| 11 | A | 543 | U | C2-N3 | -5.68 | 1.33 | 1.37 |
| 11 | A | 289 | G | C6-N1 | -5.68 | 1.35 | 1.39 |
| 11 | A | 269 | C | C4-C5 | -5.67 | 1.38 | 1.43 |
| 11 | A | 234 | C | C2-N3 | -5.65 | 1.31 | 1.35 |
| 11 | A | 196 | A | N3-C4 | -5.64 | 1.31 | 1.34 |
| 11 | A | 380 | G | C5-C4 | -5.64 | 1.34 | 1.38 |
| 11 | A | 271 | C | N1-C2 | -5.63 | 1.34 | 1.40 |
| 11 | A | 52 | C | N3-C4 | -5.62 | 1.30 | 1.33 |
| 11 | A | 199 | A | C8-N7 | -5.62 | 1.27 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 11 | A | 451 | A | N3-C4 | -5.62 | 1.31 | 1.34 |
| 11 | A | 61 | G | N1-C2 | -5.61 | 1.33 | 1.37 |
| 11 | A | 448 | A | N9-C4 | -5.61 | 1.34 | 1.37 |
| 11 | A | 323 | U | N3-C4 | -5.61 | 1.33 | 1.38 |
| 11 | A | 45 | G | C5-C6 | -5.60 | 1.36 | 1.42 |
| 11 | A | 116 | A | C6-N1 | -5.60 | 1.31 | 1.35 |
| 11 | A | 326 | G | C6-N1 | -5.60 | 1.35 | 1.39 |
| 11 | A | 482 | A | N9-C4 | -5.60 | 1.34 | 1.37 |
| 11 | A | 877 | G | C5-C4 | -5.59 | 1.34 | 1.38 |
| 11 | A | 175 | C | C2-N3 | -5.59 | 1.31 | 1.35 |
| 11 | A | 327 | A | C5-C4 | -5.59 | 1.34 | 1.38 |
| 11 | A | 395 | C | C2-N3 | -5.58 | 1.31 | 1.35 |
| 11 | A | 384 | G | C5-C4 | -5.58 | 1.34 | 1.38 |
| 11 | A | 451 | A | N7-C5 | -5.56 | 1.35 | 1.39 |
| 11 | A | 195 | A | N9-C4 | -5.55 | 1.34 | 1.37 |
| 11 | A | 326 | G | N1-C2 | -5.55 | 1.33 | 1.37 |
| 11 | A | 357 | G | C2-N3 | -5.55 | 1.28 | 1.32 |
| 11 | A | 143 | A | N9-C4 | -5.55 | 1.34 | 1.37 |
| 11 | A | 258 | G | C6-N1 | -5.55 | 1.35 | 1.39 |
| 11 | A | 329 | A | C8-N7 | -5.55 | 1.27 | 1.31 |
| 11 | A | 547 | A | C5-C4 | -5.54 | 1.34 | 1.38 |
| 11 | A | 257 | G | C2-N3 | -5.54 | 1.28 | 1.32 |
| 11 | A | 58 | C | N1-C6 | -5.54 | 1.33 | 1.37 |
| 11 | A | 222 | C | N3-C4 | -5.53 | 1.30 | 1.33 |
| 11 | A | 232 | G | C5-C4 | -5.52 | 1.34 | 1.38 |
| 11 | A | 107 | G | N7-C5 | -5.51 | 1.35 | 1.39 |
| 11 | A | 376 | G | C6-N1 | -5.51 | 1.35 | 1.39 |
| 11 | A | 386 | C | N3-C4 | -5.51 | 1.30 | 1.33 |
| 11 | A | 186 | C | N3-C4 | -5.50 | 1.30 | 1.33 |
| 11 | A | 374 | A | C8-N7 | -5.50 | 1.27 | 1.31 |
| 11 | A | 757 | U | C2-N3 | -5.50 | 1.33 | 1.37 |
| 11 | A | 314 | C | C4-C5 | -5.49 | 1.38 | 1.43 |
| 11 | A | 610 | U | C2-N3 | -5.48 | 1.33 | 1.37 |
| 11 | A | 69 | G | C6-N1 | -5.48 | 1.35 | 1.39 |
| 11 | A | 315 | A | C8-N7 | -5.48 | 1.27 | 1.31 |
| 11 | A | 222 | C | C4-C5 | -5.47 | 1.38 | 1.43 |
| 11 | A | 42 | G | N1-C2 | -5.47 | 1.33 | 1.37 |
| 11 | A | 550 | G | C5-C4 | -5.47 | 1.34 | 1.38 |
| 11 | A | 117 | G | C8-N7 | -5.46 | 1.27 | 1.30 |
| 11 | A | 332 | G | N7-C5 | -5.46 | 1.35 | 1.39 |
| 11 | A | 41 | G | N1-C2 | -5.46 | 1.33 | 1.37 |
| 11 | A | 108 | G | N3-C4 | -5.46 | 1.31 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11 | A | 102 | G | C2-N3 | -5.45 | 1.28 | 1.32 |
| 11 | A | 758 | C | N1-C6 | -5.45 | 1.33 | 1.37 |
| 11 | A | 107 | G | C2-N3 | -5.44 | 1.28 | 1.32 |
| 11 | A | 122 | G | C5-C4 | -5.44 | 1.34 | 1.38 |
| 11 | A | 489 | C | N1-C6 | -5.44 | 1.33 | 1.37 |
| 11 | A | 131 | A | N3-C4 | -5.43 | 1.31 | 1.34 |
| 11 | A | 171 | A | N7-C5 | -5.43 | 1.35 | 1.39 |
| 11 | A | 197 | A | C5-C4 | -5.43 | 1.34 | 1.38 |
| 11 | A | 361 | G | C5-C4 | -5.42 | 1.34 | 1.38 |
| 11 | A | 273 | U | C2-N3 | -5.42 | 1.33 | 1.37 |
| 11 | A | 228 | A | N7-C5 | -5.42 | 1.35 | 1.39 |
| 7 | P | 17 | TYR | CD1-CE1 | -5.42 | 1.31 | 1.39 |
| 11 | A | 64 | G | C5-C4 | -5.42 | 1.34 | 1.38 |
| 11 | A | 45 | G | N1-C2 | -5.41 | 1.33 | 1.37 |
| 11 | A | 62 | U | C2-N3 | -5.41 | 1.33 | 1.37 |
| 11 | A | 386 | C | N1-C6 | -5.41 | 1.33 | 1.37 |
| 11 | A | 184 | G | C2-N3 | -5.41 | 1.28 | 1.32 |
| 11 | A | 539 | A | N9-C4 | -5.40 | 1.34 | 1.37 |
| 11 | A | 481 | G | N7-C5 | -5.39 | 1.36 | 1.39 |
| 11 | A | 331 | G | C5-C4 | -5.39 | 1.34 | 1.38 |
| 11 | A | 502 | A | C6-N1 | -5.38 | 1.31 | 1.35 |
| 11 | A | 319 | G | C6-N1 | -5.38 | 1.35 | 1.39 |
| 11 | A | 40 | C | N3-C4 | -5.37 | 1.30 | 1.33 |
| 11 | A | 270 | A | C6-N1 | -5.37 | 1.31 | 1.35 |
| 11 | A | 143 | A | C8-N7 | -5.37 | 1.27 | 1.31 |
| 11 | A | 261 | U | C2-N3 | -5.36 | 1.33 | 1.37 |
| 11 | A | 402 | G | C5-C6 | -5.36 | 1.36 | 1.42 |
| 11 | A | 373 | A | C6-N1 | -5.36 | 1.31 | 1.35 |
| 11 | A | 501 | C | C2-N3 | -5.35 | 1.31 | 1.35 |
| 11 | A | 371 | A | C8-N7 | -5.35 | 1.27 | 1.31 |
| 11 | A | 39 | G | C6-N1 | -5.34 | 1.35 | 1.39 |
| 11 | A | 111 | G | C8-N7 | -5.34 | 1.27 | 1.30 |
| 11 | A | 391 | G | C5-C6 | -5.34 | 1.37 | 1.42 |
| 11 | A | 104 | G | C5-C4 | -5.33 | 1.34 | 1.38 |
| 11 | A | 353 | A | C5-C6 | -5.33 | 1.36 | 1.41 |
| 11 | A | 259 | G | C6-N1 | -5.33 | 1.35 | 1.39 |
| 11 | A | 378 | G | N1-C2 | -5.32 | 1.33 | 1.37 |
| 11 | A | 622 | A | N9-C4 | -5.32 | 1.34 | 1.37 |
| 11 | A | 289 | G | C5-C4 | -5.30 | 1.34 | 1.38 |
| 11 | A | 352 | C | C2-N3 | -5.30 | 1.31 | 1.35 |
| 11 | A | 545 | C | N3-C4 | -5.30 | 1.30 | 1.33 |
| 11 | A | 310 | G | C5-C4 | -5.30 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 11 | A | 362 | G | N9-C4 | -5.30 | 1.33 | 1.38 |
| 11 | A | 35 | G | C6-N1 | -5.29 | 1.35 | 1.39 |
| 11 | A | 44 | A | N7-C5 | -5.29 | 1.36 | 1.39 |
| 11 | A | 120 | A | N9-C4 | -5.29 | 1.34 | 1.37 |
| 11 | A | 279 | A | N9-C4 | -5.29 | 1.34 | 1.37 |
| 11 | A | 304 | U | C2-N3 | -5.28 | 1.34 | 1.37 |
| 11 | A | 142 | G | C6-N1 | -5.28 | 1.35 | 1.39 |
| 11 | A | 338 | A | N9-C4 | -5.28 | 1.34 | 1.37 |
| 11 | A | 147 | G | C8-N7 | -5.27 | 1.27 | 1.30 |
| 11 | A | 54 | C | C4-C5 | -5.27 | 1.38 | 1.43 |
| 11 | A | 123 | U | C2-N3 | -5.26 | 1.34 | 1.37 |
| 11 | A | 175 | C | N1-C6 | -5.26 | 1.33 | 1.37 |
| 11 | A | 313 | A | C2-N3 | -5.26 | 1.28 | 1.33 |
| 11 | A | 357 | G | C5-C4 | -5.25 | 1.34 | 1.38 |
| 11 | A | 378 | G | N3-C4 | -5.25 | 1.31 | 1.35 |
| 11 | A | 393 | A | C8-N7 | -5.25 | 1.27 | 1.31 |
| 11 | A | 149 | A | N9-C4 | -5.24 | 1.34 | 1.37 |
| 11 | A | 391 | G | C5-C4 | -5.24 | 1.34 | 1.38 |
| 11 | A | 331 | G | C2-N3 | -5.23 | 1.28 | 1.32 |
| 11 | A | 357 | G | C8-N7 | -5.23 | 1.27 | 1.30 |
| 11 | A | 41 | G | C8-N7 | -5.23 | 1.27 | 1.30 |
| 11 | A | 175 | C | C4-C5 | -5.23 | 1.38 | 1.43 |
| 11 | A | 389 | A | N9-C8 | -5.22 | 1.33 | 1.37 |
| 11 | A | 104 | G | C6-N1 | -5.22 | 1.35 | 1.39 |
| 11 | A | 224 | U | C2-N3 | -5.22 | 1.34 | 1.37 |
| 11 | A | 550 | G | C2-N3 | -5.21 | 1.28 | 1.32 |
| 11 | A | 131 | A | C6-N1 | -5.21 | 1.31 | 1.35 |
| 11 | A | 45 | G | C8-N7 | -5.20 | 1.27 | 1.30 |
| 11 | A | 220 | G | C5-C4 | -5.19 | 1.34 | 1.38 |
| 11 | A | 387 | U | N3-C4 | -5.19 | 1.33 | 1.38 |
| 11 | A | 196 | A | C5-C4 | -5.18 | 1.35 | 1.38 |
| 11 | A | 265 | G | C5-C4 | -5.18 | 1.34 | 1.38 |
| 11 | A | 223 | A | C5-C4 | -5.18 | 1.35 | 1.38 |
| 11 | A | 313 | A | C5-C4 | -5.18 | 1.35 | 1.38 |
| 11 | A | 617 | G | C8-N7 | -5.18 | 1.27 | 1.30 |
| 11 | A | 142 | G | C5-C4 | -5.17 | 1.34 | 1.38 |
| 11 | A | 174 | A | N9-C4 | -5.17 | 1.34 | 1.37 |
| 11 | A | 354 | G | N3-C4 | -5.16 | 1.31 | 1.35 |
| 11 | A | 59 | A | C5-C4 | -5.16 | 1.35 | 1.38 |
| 11 | A | 199 | A | C6-N1 | -5.16 | 1.31 | 1.35 |
| 11 | A | 368 | U | C2-N3 | -5.15 | 1.34 | 1.37 |
| 11 | A | 502 | A | C5-C6 | -5.15 | 1.36 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 11 | A | 487 | A | N7-C5 | -5.15 | 1.36 | 1.39 |
| 11 | A | 326 | G | N7-C5 | -5.15 | 1.36 | 1.39 |
| 11 | A | 114 | U | C2-N3 | -5.14 | 1.34 | 1.37 |
| 11 | A | 40 | C | C2-N3 | -5.14 | 1.31 | 1.35 |
| 11 | A | 174 | A | N3-C4 | -5.14 | 1.31 | 1.34 |
| 11 | A | 323 | U | C5-C6 | -5.14 | 1.29 | 1.34 |
| 11 | A | 333 | U | C2-N3 | -5.14 | 1.34 | 1.37 |
| 11 | A | 391 | G | N9-C8 | -5.13 | 1.34 | 1.37 |
| 11 | A | 172 | A | C6-N1 | -5.13 | 1.31 | 1.35 |
| 11 | A | 385 | C | N1-C6 | -5.13 | 1.34 | 1.37 |
| 11 | A | 510 | A | N9-C4 | -5.12 | 1.34 | 1.37 |
| 11 | A | 141 | G | N7-C5 | -5.12 | 1.36 | 1.39 |
| 11 | A | 448 | A | N3-C4 | -5.12 | 1.31 | 1.34 |
| 11 | A | 450 | G | C2-N3 | -5.12 | 1.28 | 1.32 |
| 11 | A | 197 | A | N3-C4 | -5.12 | 1.31 | 1.34 |
| 11 | A | 628 | G | N1-C2 | -5.12 | 1.33 | 1.37 |
| 11 | A | 388 | G | C8-N7 | -5.11 | 1.27 | 1.30 |
| 11 | A | 482 | A | C8-N7 | -5.11 | 1.27 | 1.31 |
| 11 | A | 176 | C | N3-C4 | -5.11 | 1.30 | 1.33 |
| 11 | A | 484 | G | C8-N7 | -5.11 | 1.27 | 1.30 |
| 11 | A | 36 | C | N3-C4 | -5.11 | 1.30 | 1.33 |
| 11 | A | 482 | A | C6-N1 | -5.10 | 1.31 | 1.35 |
| 11 | A | 64 | G | N1-C2 | -5.10 | 1.33 | 1.37 |
| 11 | A | 382 | A | C5-C4 | -5.10 | 1.35 | 1.38 |
| 11 | A | 610 | U | C2-O2 | -5.10 | 1.17 | 1.22 |
| 11 | A | 181 | A | C5-C6 | -5.10 | 1.36 | 1.41 |
| 11 | A | 481 | G | N9-C8 | -5.10 | 1.34 | 1.37 |
| 11 | A | 127 | G | C5-C4 | -5.09 | 1.34 | 1.38 |
| 11 | A | 484 | G | C2-N3 | -5.09 | 1.28 | 1.32 |
| 11 | A | 320 | A | C2-N3 | -5.09 | 1.28 | 1.33 |
| 11 | A | 126 | G | C6-N1 | -5.09 | 1.35 | 1.39 |
| 11 | A | 105 | G | N9-C4 | -5.08 | 1.33 | 1.38 |
| 11 | A | 240 | G | C5-C4 | -5.08 | 1.34 | 1.38 |
| 11 | A | 324 | G | C6-N1 | -5.08 | 1.35 | 1.39 |
| 11 | A | 547 | A | N9-C4 | -5.08 | 1.34 | 1.37 |
| 11 | A | 402 | G | C2-N3 | -5.08 | 1.28 | 1.32 |
| 11 | A | 227 | G | C2-N3 | -5.07 | 1.28 | 1.32 |
| 11 | A | 324 | G | N9-C8 | -5.07 | 1.34 | 1.37 |
| 11 | A | 375 | U | C2-N3 | -5.07 | 1.34 | 1.37 |
| 11 | A | 393 | A | C6-N1 | -5.07 | 1.31 | 1.35 |
| 11 | A | 377 | G | N3-C4 | -5.07 | 1.31 | 1.35 |
| 11 | A | 544 | G | C6-N1 | -5.07 | 1.36 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 11 | A | 326 | G | C2-N3 | -5.06 | 1.28 | 1.32 |
| 11 | A | 254 | G | C6-N1 | -5.05 | 1.36 | 1.39 |
| 11 | A | 450 | G | N9-C8 | -5.05 | 1.34 | 1.37 |
| 11 | A | 270 | A | C5-C6 | -5.05 | 1.36 | 1.41 |
| 11 | A | 324 | G | C2-N3 | -5.04 | 1.28 | 1.32 |
| 11 | A | 360 | G | N7-C5 | -5.04 | 1.36 | 1.39 |
| 11 | A | 383 | A | N7-C5 | -5.04 | 1.36 | 1.39 |
| 11 | A | 327 | A | N9-C8 | -5.04 | 1.33 | 1.37 |
| 11 | A | 544 | G | C5-C4 | -5.03 | 1.34 | 1.38 |
| 11 | A | 621 | A | C5-C6 | -5.03 | 1.36 | 1.41 |
| 11 | A | 68 | G | C2-N3 | -5.03 | 1.28 | 1.32 |
| 11 | A | 111 | G | N9-C8 | -5.03 | 1.34 | 1.37 |
| 11 | A | 193 | C | N3-C4 | -5.03 | 1.30 | 1.33 |
| 11 | A | 538 | G | C6-N1 | -5.03 | 1.36 | 1.39 |
| 11 | A | 151 | A | N9-C4 | -5.02 | 1.34 | 1.37 |
| 11 | A | 51 | A | N7-C5 | -5.02 | 1.36 | 1.39 |
| 11 | A | 313 | A | C8-N7 | -5.02 | 1.28 | 1.31 |
| 11 | A | 380 | G | N9-C8 | -5.02 | 1.34 | 1.37 |
| 11 | A | 130 | A | C5-C4 | -5.02 | 1.35 | 1.38 |
| 11 | A | 447 | G | N9-C8 | -5.02 | 1.34 | 1.37 |
| 11 | A | 358 | U | C2-N3 | -5.01 | 1.34 | 1.37 |
| 11 | A | 376 | G | N7-C5 | -5.01 | 1.36 | 1.39 |
| 11 | A | 265 | G | C8-N7 | -5.01 | 1.27 | 1.30 |
| 11 | A | 367 | U | C2-N3 | -5.01 | 1.34 | 1.37 |
| 11 | A | 374 | A | C6-N1 | -5.01 | 1.32 | 1.35 |
| 11 | A | 454 | G | C5-C4 | -5.01 | 1.34 | 1.38 |
| 11 | A | 51 | A | N9-C8 | -5.01 | 1.33 | 1.37 |
| 11 | A | 391 | G | C6-O6 | -5.01 | 1.19 | 1.24 |
| 11 | A | 401 | C | C4-C5 | -5.00 | 1.39 | 1.43 |
| 11 | A | 452 | A | N7-C5 | -5.00 | 1.36 | 1.39 |

All (132) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 11 | A | 108 | G | C4-C5-N7 | 15.57 | 117.03 | 110.80 |
| 11 | A | 108 | G | C5-N7-C8 | -12.91 | 97.84 | 104.30 |
| 11 | A | 108 | G | C6-C5-N7 | -12.81 | 122.71 | 130.40 |
| 11 | A | 452 | A | C2-N3-C4 | -10.97 | 105.11 | 110.60 |
| 11 | A | 452 | A | N3-C4-C5 | 10.44 | 134.11 | 126.80 |
| 11 | A | 452 | A | N3-C4-N9 | -10.38 | 119.09 | 127.40 |
| 11 | A | 108 | G | N1-C6-O6 | 10.31 | 126.08 | 119.90 |
| 11 | A | 182 | A | O4'-C1'-N9 | 9.96 | 116.16 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11 | A | 372 | C | C6-N1-C2 | -9.63 | 116.45 | 120.30 |
| 11 | A | 108 | G | C5-C6-O6 | -9.15 | 123.11 | 128.60 |
| 11 | A | 181 | A | O4'-C1'-N9 | 9.10 | 115.48 | 108.20 |
| 11 | A | 182 | A | C5-N7-C8 | -8.86 | 99.47 | 103.90 |
| 11 | A | 353 | A | C5-N7-C8 | -8.54 | 99.63 | 103.90 |
| 11 | A | 108 | G | N7-C8-N9 | 8.36 | 117.28 | 113.10 |
| 11 | A | 511 | C | N1-C2-O2 | -8.33 | 113.90 | 118.90 |
| 11 | A | 462 | G | C4-N9-C1' | 8.29 | 137.28 | 126.50 |
| 11 | A | 462 | G | C8-N9-C1' | -8.04 | 116.55 | 127.00 |
| 11 | A | 108 | G | C4-N9-C1' | 8.00 | 136.90 | 126.50 |
| 11 | A | 610 | U | N3-C2-O2 | -7.93 | 116.65 | 122.20 |
| 11 | A | 736 | C | N3-C2-O2 | -7.80 | 116.44 | 121.90 |
| 11 | A | 266 | G | N9-C4-C5 | -7.71 | 102.32 | 105.40 |
| 11 | A | 108 | G | N9-C4-C5 | -7.70 | 102.32 | 105.40 |
| 11 | A | 108 | G | C8-N9-C1' | -7.62 | 117.09 | 127.00 |
| 11 | A | 182 | A | N7-C8-N9 | 7.55 | 117.58 | 113.80 |
| 11 | A | 396 | C | N3-C4-C5 | 7.49 | 124.90 | 121.90 |
| 11 | A | 708 | C | N3-C2-O2 | -7.38 | 116.73 | 121.90 |
| 11 | A | 383 | A | C8-N9-C4 | -7.22 | 102.91 | 105.80 |
| 11 | A | 383 | A | N7-C8-N9 | 7.20 | 117.40 | 113.80 |
| 11 | A | 736 | C | N1-C2-O2 | 7.10 | 123.16 | 118.90 |
| 11 | A | 353 | A | C4-C5-N7 | 7.06 | 114.23 | 110.70 |
| 11 | A | 462 | G | C6-C5-N7 | -7.06 | 126.16 | 130.40 |
| 11 | A | 181 | A | C8-N9-C4 | 7.05 | 108.62 | 105.80 |
| 11 | A | 266 | G | C8-N9-C4 | 6.96 | 109.18 | 106.40 |
| 11 | A | 314 | C | N3-C4-C5 | 6.87 | 124.65 | 121.90 |
| 11 | A | 452 | A | C6-N1-C2 | 6.84 | 122.71 | 118.60 |
| 11 | A | 517 | G | C5-C6-O6 | -6.81 | 124.52 | 128.60 |
| 11 | A | 279 | A | C2-N3-C4 | -6.80 | 107.20 | 110.60 |
| 11 | A | 496 | A | O4'-C1'-N9 | 6.68 | 113.54 | 108.20 |
| 11 | A | 353 | A | O4'-C1'-N9 | 6.62 | 113.50 | 108.20 |
| 11 | A | 332 | G | C5-C6-O6 | -6.58 | 124.65 | 128.60 |
| 11 | A | 328 | C | P-O3'-C3' | 6.54 | 127.55 | 119.70 |
| 11 | A | 462 | G | C4-C5-N7 | 6.46 | 113.38 | 110.80 |
| 11 | A | 737 | C | N3-C2-O2 | -6.41 | 117.41 | 121.90 |
| 11 | A | 416 | G | C4'-C3'-O3' | 6.30 | 125.61 | 113.00 |
| 11 | A | 269 | C | N3-C4-C5 | 6.28 | 124.41 | 121.90 |
| 11 | A | 152 | A | C5-N7-C8 | -6.27 | 100.77 | 103.90 |
| 11 | A | 354 | G | C4-C5-N7 | 6.24 | 113.30 | 110.80 |
| 11 | A | 416 | G | C3'-C2'-C1' | 6.19 | 106.45 | 101.50 |
| 11 | A | 915 | A | N1-C6-N6 | -6.19 | 114.89 | 118.60 |
| 11 | A | 266 | G | C5-C6-N1 | -6.17 | 108.41 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11 | A | 462 | G | N7-C8-N9 | 6.13 | 116.17 | 113.10 |
| 11 | A | 181 | A | N9-C4-C5 | -6.09 | 103.36 | 105.80 |
| 11 | A | 353 | A | C2-N3-C4 | -6.06 | 107.57 | 110.60 |
| 11 | A | 332 | G | N1-C6-O6 | 6.04 | 123.52 | 119.90 |
| 11 | A | 786 | G | N1-C6-O6 | -6.03 | 116.28 | 119.90 |
| 11 | A | 465 | A | C8-N9-C4 | -6.03 | 103.39 | 105.80 |
| 11 | A | 465 | A | C3'-C2'-C1' | -6.02 | 96.68 | 101.50 |
| 11 | A | 708 | C | N1-C2-O2 | 5.99 | 122.50 | 118.90 |
| 11 | A | 538 | G | C4-C5-N7 | 5.98 | 113.19 | 110.80 |
| 11 | A | 124 | C | C6-N1-C2 | -5.97 | 117.91 | 120.30 |
| 11 | A | 452 | A | C4-C5-C6 | -5.96 | 114.02 | 117.00 |
| 11 | A | 543 | U | N3-C2-O2 | -5.96 | 118.03 | 122.20 |
| 11 | A | 311 | C | C6-N1-C2 | -5.93 | 117.93 | 120.30 |
| 11 | A | 462 | G | C5-N7-C8 | -5.85 | 101.38 | 104.30 |
| 11 | A | 462 | G | N9-C4-C5 | -5.83 | 103.07 | 105.40 |
| 11 | A | 403 | C | N3-C4-C5 | 5.82 | 124.23 | 121.90 |
| 11 | A | 610 | U | C6-N1-C2 | -5.81 | 117.52 | 121.00 |
| 11 | A | 876 | C | N3-C4-C5 | 5.80 | 124.22 | 121.90 |
| 11 | A | 372 | C | N3-C4-C5 | -5.78 | 119.59 | 121.90 |
| 11 | A | 416 | G | N9-C1'-C2' | -5.78 | 105.65 | 112.00 |
| 11 | A | 37 | U | C2-N3-C4 | -5.77 | 123.54 | 127.00 |
| 11 | A | 193 | C | C5-C6-N1 | -5.75 | 118.13 | 121.00 |
| 11 | A | 52 | C | C6-N1-C2 | -5.70 | 118.02 | 120.30 |
| 11 | A | 474 | G | O4'-C1'-N9 | 5.70 | 112.76 | 108.20 |
| 11 | A | 517 | G | C4-C5-N7 | 5.68 | 113.07 | 110.80 |
| 11 | A | 266 | G | N1-C6-O6 | 5.68 | 123.31 | 119.90 |
| 11 | A | 494 | G | C4-C5-N7 | 5.68 | 113.07 | 110.80 |
| 11 | A | 266 | G | C8-N9-C1' | -5.64 | 119.67 | 127.00 |
| 11 | A | 147 | G | N9-C4-C5 | -5.63 | 103.15 | 105.40 |
| 11 | A | 219 | U | N3-C4-O4 | -5.61 | 115.47 | 119.40 |
| 11 | A | 182 | A | C4-C5-N7 | 5.60 | 113.50 | 110.70 |
| 11 | A | 121 | U | N1-C2-O2 | 5.59 | 126.71 | 122.80 |
| 11 | A | 355 | C | N3-C4-N4 | -5.58 | 114.09 | 118.00 |
| 11 | A | 219 | U | C2-N1-C1' | -5.55 | 111.04 | 117.70 |
| 11 | A | 322 | C | C5-C6-N1 | -5.54 | 118.23 | 121.00 |
| 11 | A | 219 | U | C5-C4-O4 | 5.51 | 129.20 | 125.90 |
| 11 | A | 438 | U | O4'-C1'-N1 | 5.48 | 112.59 | 108.20 |
| 11 | A | 460 | A | N9-C4-C5 | -5.46 | 103.61 | 105.80 |
| 11 | A | 386 | C | N3-C4-C5 | 5.45 | 124.08 | 121.90 |
| 11 | A | 452 | A | C5-C6-N6 | 5.45 | 128.06 | 123.70 |
| 11 | A | 617 | G | C8-N9-C4 | 5.44 | 108.58 | 106.40 |
| 11 | A | 148 | G | C5-N7-C8 | -5.42 | 101.59 | 104.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11 | A | 465 | A | N9-C1'-C2' | -5.41 | 106.05 | 112.00 |
| 11 | A | 269 | C | C4-C5-C6 | -5.41 | 114.70 | 117.40 |
| 11 | A | 108 | G | N9-C1'-C2' | -5.40 | 106.06 | 112.00 |
| 11 | A | 365 | U | O4'-C1'-N1 | 5.40 | 112.52 | 108.20 |
| 11 | A | 403 | C | C2-N3-C4 | -5.39 | 117.20 | 119.90 |
| 11 | A | 786 | G | C5-C6-O6 | 5.38 | 131.83 | 128.60 |
| 11 | A | 221 | C | N1-C2-O2 | 5.36 | 122.12 | 118.90 |
| 11 | A | 109 | A | N1-C2-N3 | -5.35 | 126.62 | 129.30 |
| 11 | A | 69 | G | C8-N9-C1' | -5.33 | 120.08 | 127.00 |
| 11 | A | 103 | U | N3-C2-O2 | -5.29 | 118.50 | 122.20 |
| 11 | A | 175 | C | N3-C4-C5 | 5.29 | 124.02 | 121.90 |
| 11 | A | 737 | C | C6-N1-C2 | -5.29 | 118.19 | 120.30 |
| 11 | A | 517 | G | N1-C6-O6 | 5.28 | 123.07 | 119.90 |
| 11 | A | 54 | C | N3-C4-C5 | 5.28 | 124.01 | 121.90 |
| 11 | A | 251 | G | C5-C6-O6 | 5.27 | 131.76 | 128.60 |
| 11 | A | 69 | G | N9-C4-C5 | -5.26 | 103.30 | 105.40 |
| 11 | A | 365 | U | C2-N1-C1' | 5.25 | 124.00 | 117.70 |
| 11 | A | 467 | U | C2-N1-C1' | 5.24 | 123.98 | 117.70 |
| 11 | A | 332 | G | C4-C5-N7 | 5.23 | 112.89 | 110.80 |
| 11 | A | 494 | G | C5-C6-O6 | -5.22 | 125.47 | 128.60 |
| 11 | A | 320 | A | C8-N9-C4 | 5.22 | 107.89 | 105.80 |
| 11 | A | 465 | A | C4'-C3'-O3' | 5.21 | 123.41 | 113.00 |
| 11 | A | 121 | U | N3-C2-O2 | -5.20 | 118.56 | 122.20 |
| 11 | A | 332 | G | N9-C4-C5 | -5.20 | 103.32 | 105.40 |
| 11 | A | 467 | U | N3-C2-O2 | -5.18 | 118.57 | 122.20 |
| 11 | A | 356 | A | O4'-C1'-N9 | 5.17 | 112.33 | 108.20 |
| 11 | A | 266 | G | C6-C5-N7 | -5.15 | 127.31 | 130.40 |
| 11 | A | 67 | C | C2-N3-C4 | -5.12 | 117.34 | 119.90 |
| 11 | A | 40 | C | N3-C4-C5 | 5.12 | 123.95 | 121.90 |
| 11 | A | 353 | A | N7-C8-N9 | 5.11 | 116.36 | 113.80 |
| 11 | A | 394 | G | C5-C6-N1 | 5.11 | 114.05 | 111.50 |
| 11 | A | 183 | C | P-O3'-C3' | 5.10 | 125.82 | 119.70 |
| 11 | A | 586 | C | N3-C4-C5 | 5.09 | 123.94 | 121.90 |
| 11 | A | 372 | C | C5-C4-N4 | 5.08 | 123.76 | 120.20 |
| 11 | A | 109 | A | N9-C4-C5 | -5.08 | 103.77 | 105.80 |
| 11 | A | 71 | A | C3'-C2'-C1' | 5.05 | 105.54 | 101.50 |
| 11 | A | 379 | C | N3-C4-C5 | 5.05 | 123.92 | 121.90 |
| 11 | A | 322 | C | C6-N1-C2 | 5.04 | 122.32 | 120.30 |
| 11 | A | 354 | G | C2-N3-C4 | -5.02 | 109.39 | 111.90 |
| 11 | A | 54 | C | O4'-C1'-N1 | 5.02 | 112.21 | 108.20 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | D | 1643 | 0 | 1710 | 120 | 0 |
| 2 | F | 817 | 0 | 808 | 62 | 0 |
| 3 | H | 979 | 0 | 1034 | 50 | 0 |
| 4 | K | 702 | 0 | 702 | 41 | 0 |
| 5 | L | 955 | 0 | 1019 | 61 | 0 |
| 6 | O | 716 | 0 | 742 | 50 | 0 |
| 7 | P | 649 | 0 | 666 | 25 | 0 |
| 8 | Q | 648 | 0 | 691 | 33 | 0 |
| 9 | R | 407 | 0 | 438 | 26 | 0 |
| 10 | T | 665 | 0 | 714 | 23 | 0 |
| 11 | A | 20700 | 0 | 10405 | 711 | 0 |
| 12 | A | 337 | 0 | 0 | 22 | 0 |
| 12 | D | 6 | 0 | 0 | 0 | 0 |
| 12 | L | 4 | 0 | 0 | 0 | 0 |
| 12 | P | 18 | 0 | 0 | 3 | 0 |
| 12 | Q | 3 | 0 | 0 | 1 | 0 |
| 12 | T | 6 | 0 | 0 | 1 | 0 |
| All | All | 29255 | 0 | 18929 | 1094 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (1094) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|-----------------|--------------------------|-------------------|
| 1:D:31:CYS:SG | 11:A:429:U:H5'' | 1.50 | 1.52 |
| 11:A:26:A:N6 | 11:A:558:G:N3 | 1.91 | 1.17 |
| 1:D:8:LEU:CD2 | 11:A:429:U:H3' | 1.73 | 1.16 |
| 1:D:31:CYS:SG | 11:A:429:U:C5' | 2.36 | 1.12 |
| 11:A:411:A:C2 | 11:A:430:A:N6 | 2.17 | 1.11 |
| 1:D:9:LYS:HG3 | 1:D:37:PRO:CB | 1.80 | 1.11 |
| 2:F:2:ARG:HG2 | 2:F:92:THR:CG2 | 1.82 | 1.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:D:8:LEU:HD22 | 11:A:429:U:C3' | 1.84 | 1.07 |
| 1:D:8:LEU:HD23 | 1:D:31:CYS:SG | 1.95 | 1.07 |
| 1:D:33:ILE:HG22 | 1:D:34:GLU:H | 1.17 | 1.07 |
| 11:A:411:A:N1 | 11:A:430:A:N6 | 2.04 | 1.06 |
| 6:O:47:LYS:HE2 | 11:A:808:C:OP1 | 1.57 | 1.04 |
| 6:O:38:LEU:HD22 | 6:O:55:LEU:HD13 | 1.36 | 1.02 |
| 8:Q:13:SER:OG | 8:Q:15:LYS:HD3 | 1.59 | 1.01 |
| 1:D:112:GLU:OE2 | 1:D:153:ARG:HD2 | 1.60 | 1.01 |
| 11:A:687:A:H62 | 11:A:703:G:N2 | 1.57 | 1.01 |
| 2:F:20:GLY:O | 2:F:24:ARG:HG3 | 1.62 | 0.99 |
| 5:L:66:ILE:HD12 | 5:L:96:THR:HG21 | 1.46 | 0.98 |
| 11:A:76:G:H1 | 11:A:93:U:H3 | 1.09 | 0.97 |
| 11:A:448:A:N7 | 11:A:486:U:N3 | 2.13 | 0.97 |
| 11:A:663:A:H61 | 11:A:742:G:H1 | 1.13 | 0.96 |
| 11:A:836:G:H1 | 11:A:850:U:H3 | 0.99 | 0.96 |
| 11:A:444:G:N2 | 11:A:490:C:O2 | 1.98 | 0.96 |
| 11:A:411:A:N6 | 11:A:430:A:N7 | 2.13 | 0.96 |
| 1:D:108:ALA:H | 1:D:112:GLU:HG2 | 1.32 | 0.95 |
| 11:A:457:G:N2 | 11:A:475:C:O2 | 1.98 | 0.95 |
| 11:A:335:C:HO2' | 11:A:336:A:H8 | 0.96 | 0.95 |
| 11:A:148:G:H1 | 11:A:174:A:N6 | 1.62 | 0.94 |
| 2:F:2:ARG:HG2 | 2:F:92:THR:HG21 | 1.50 | 0.94 |
| 11:A:148:G:H1 | 11:A:174:A:H61 | 0.97 | 0.94 |
| 11:A:687:A:N6 | 11:A:703:G:H21 | 1.66 | 0.93 |
| 11:A:444:G:N1 | 11:A:490:C:N3 | 2.15 | 0.93 |
| 1:D:1:ALA:HB3 | 11:A:547:A:OP2 | 1.69 | 0.93 |
| 11:A:658:C:O2 | 11:A:748:G:N2 | 2.02 | 0.93 |
| 11:A:94:G:N2 | 11:A:97:G:N7 | 2.17 | 0.92 |
| 1:D:98:ASP:OD1 | 1:D:99:ASN:N | 2.02 | 0.92 |
| 11:A:687:A:H62 | 11:A:703:G:H21 | 0.94 | 0.92 |
| 11:A:187:G:N2 | 11:A:190:A:N7 | 2.20 | 0.90 |
| 11:A:462:G:N1 | 11:A:470:C:N3 | 2.20 | 0.90 |
| 6:O:38:LEU:HD23 | 6:O:55:LEU:HB2 | 1.53 | 0.90 |
| 11:A:207:C:H5 | 12:A:1732:HOH:O | 1.54 | 0.89 |
| 3:H:42:GLU:OE2 | 3:H:44:PHE:HD2 | 1.55 | 0.88 |
| 11:A:839:C:O2 | 11:A:847:G:N2 | 2.07 | 0.86 |
| 11:A:411:A:H2 | 11:A:430:A:N6 | 1.71 | 0.86 |
| 10:T:9:ARG:NH2 | 11:A:107:G:N7 | 2.23 | 0.85 |
| 1:D:9:LYS:HG3 | 1:D:37:PRO:HB2 | 1.55 | 0.85 |
| 1:D:1:ALA:CB | 11:A:547:A:OP2 | 2.25 | 0.85 |
| 11:A:658:C:N3 | 11:A:748:G:N1 | 2.25 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 11:A:674:G:H2' | 11:A:675:A:H8 | 1.42 | 0.84 |
| 2:F:18:VAL:O | 2:F:22:ILE:HG13 | 1.77 | 0.84 |
| 11:A:839:C:N3 | 11:A:847:G:N1 | 2.24 | 0.84 |
| 11:A:682:G:H2' | 11:A:683:G:C8 | 2.13 | 0.84 |
| 11:A:515:G:OP2 | 11:A:532:A:N6 | 2.11 | 0.83 |
| 11:A:152:A:N6 | 11:A:169:C:O2 | 2.11 | 0.83 |
| 1:D:8:LEU:HD22 | 11:A:429:U:H3' | 0.89 | 0.83 |
| 11:A:202:G:HO2' | 11:A:468:A:H8 | 1.25 | 0.83 |
| 11:A:113:G:N3 | 11:A:353:A:O2' | 2.12 | 0.83 |
| 11:A:695:A:H61 | 11:A:786:G:H21 | 1.27 | 0.83 |
| 2:F:2:ARG:CG | 2:F:92:THR:CG2 | 2.57 | 0.82 |
| 11:A:559:A:H4' | 11:A:560:A:H3' | 1.61 | 0.82 |
| 8:Q:68:LYS:HG2 | 8:Q:69:THR:HG23 | 1.62 | 0.82 |
| 11:A:148:G:N2 | 11:A:174:A:N1 | 2.28 | 0.82 |
| 11:A:465:A:N6 | 11:A:468:A:N7 | 2.26 | 0.82 |
| 11:A:116:A:C2 | 12:A:1649:HOH:O | 2.32 | 0.82 |
| 2:F:2:ARG:HG2 | 2:F:92:THR:HG22 | 1.61 | 0.81 |
| 11:A:582:C:O2 | 11:A:759:A:N6 | 2.14 | 0.80 |
| 4:K:19:VAL:HG12 | 4:K:82:GLU:HB3 | 1.63 | 0.80 |
| 6:O:38:LEU:HD22 | 6:O:55:LEU:CD1 | 2.11 | 0.80 |
| 5:L:66:ILE:CD1 | 5:L:96:THR:HG21 | 2.09 | 0.80 |
| 6:O:38:LEU:CD2 | 6:O:55:LEU:HB2 | 2.12 | 0.80 |
| 1:D:8:LEU:HD23 | 11:A:429:U:H5' | 1.62 | 0.80 |
| 11:A:79:G:N2 | 11:A:90:C:O2 | 2.13 | 0.80 |
| 11:A:86:G:H1' | 11:A:87:C:H5 | 1.47 | 0.79 |
| 7:P:8:ARG:HD2 | 12:P:104:HOH:O | 1.81 | 0.79 |
| 7:P:70:ARG:O | 7:P:74:LEU:HG | 1.82 | 0.79 |
| 11:A:17:U:H2' | 11:A:18:C:C6 | 2.17 | 0.79 |
| 11:A:410:G:O6 | 11:A:429:U:O2' | 1.98 | 0.79 |
| 11:A:697:U:H1' | 11:A:785:G:H21 | 1.47 | 0.79 |
| 11:A:665:A:N7 | 11:A:724:G:O6 | 2.15 | 0.78 |
| 1:D:56:GLU:HG2 | 1:D:198:LEU:CD1 | 2.12 | 0.78 |
| 11:A:343:U:O2 | 11:A:346:G:N1 | 2.12 | 0.78 |
| 11:A:452:A:H62 | 11:A:480:U:H3 | 1.29 | 0.78 |
| 3:H:46:GLU:HB2 | 3:H:61:THR:HG23 | 1.64 | 0.78 |
| 1:D:8:LEU:CD2 | 1:D:31:CYS:SG | 2.70 | 0.78 |
| 6:O:38:LEU:CD2 | 6:O:55:LEU:HD13 | 2.12 | 0.78 |
| 11:A:79:G:N1 | 11:A:90:C:N3 | 2.26 | 0.78 |
| 1:D:146:GLU:HA | 1:D:149:LYS:HG3 | 1.64 | 0.78 |
| 11:A:766:A:H61 | 11:A:1511:G:H1' | 1.48 | 0.78 |
| 11:A:26:A:H61 | 11:A:558:G:H1' | 1.48 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 11:A:673:A:H2' | 11:A:674:G:C8 | 2.19 | 0.77 |
| 11:A:769:G:H4' | 11:A:1513:A:H4' | 1.65 | 0.77 |
| 11:A:782:A:OP1 | 11:A:1514:G:N2 | 2.18 | 0.77 |
| 8:Q:27:PHE:CZ | 8:Q:36:PHE:HB3 | 2.20 | 0.76 |
| 6:O:24:THR:HG23 | 6:O:65:LEU:HD12 | 1.66 | 0.76 |
| 11:A:116:A:H2 | 12:A:1649:HOH:O | 1.65 | 0.76 |
| 11:A:462:G:O6 | 11:A:470:C:N4 | 2.16 | 0.76 |
| 2:F:17:GLN:HG3 | 2:F:21:MET:HG2 | 1.67 | 0.76 |
| 2:F:2:ARG:CG | 2:F:92:THR:HG21 | 2.16 | 0.76 |
| 3:H:47:ASP:O | 3:H:61:THR:HG22 | 1.86 | 0.76 |
| 11:A:766:A:OP2 | 11:A:812:G:N2 | 2.18 | 0.75 |
| 11:A:830:G:N2 | 11:A:856:C:O2 | 2.13 | 0.75 |
| 11:A:768:A:N3 | 11:A:1512:U:O2' | 2.19 | 0.75 |
| 5:L:30:ARG:NH1 | 11:A:363:A:OP2 | 2.20 | 0.75 |
| 1:D:43:ARG:NH1 | 1:D:44:LYS:O | 2.19 | 0.75 |
| 2:F:29:ILE:HG21 | 2:F:64:VAL:HG21 | 1.68 | 0.75 |
| 1:D:9:LYS:HG3 | 1:D:37:PRO:HB3 | 1.67 | 0.74 |
| 1:D:58:GLN:OE1 | 1:D:61:ARG:NH1 | 2.21 | 0.74 |
| 11:A:677:U:O2 | 11:A:714:G:N2 | 2.20 | 0.74 |
| 11:A:841:C:N4 | 11:A:844:G:N7 | 2.36 | 0.74 |
| 11:A:867:G:O2' | 11:A:873:A:N1 | 2.21 | 0.74 |
| 11:A:14:U:N3 | 11:A:17:U:OP2 | 2.21 | 0.73 |
| 1:D:4:LEU:CD2 | 11:A:406:G:O5' | 2.36 | 0.73 |
| 11:A:829:G:N1 | 11:A:857:C:N3 | 2.31 | 0.73 |
| 1:D:55:ARG:NH2 | 11:A:544:G:OP1 | 2.21 | 0.73 |
| 11:A:748:G:H2' | 11:A:749:A:C8 | 2.23 | 0.73 |
| 11:A:517:G:N2 | 11:A:533:A:OP1 | 2.21 | 0.73 |
| 11:A:157:U:O2 | 11:A:164:G:O6 | 2.07 | 0.73 |
| 11:A:202:G:O2' | 11:A:468:A:H8 | 1.72 | 0.73 |
| 11:A:1391:U:H2' | 11:A:1392:G:H8 | 1.53 | 0.73 |
| 9:R:49:LYS:NZ | 11:A:836:G:OP1 | 2.22 | 0.72 |
| 3:H:110:MET:HG2 | 3:H:114:ALA:CB | 2.19 | 0.72 |
| 11:A:31:G:O2' | 11:A:48:C:N4 | 2.23 | 0.72 |
| 1:D:94:GLU:OE2 | 1:D:103:ARG:NH1 | 2.22 | 0.72 |
| 11:A:789:U:OP1 | 11:A:794:A:N6 | 2.23 | 0.72 |
| 1:D:8:LEU:HB2 | 11:A:430:A:OP1 | 1.90 | 0.71 |
| 10:T:78:LEU:O | 10:T:82:ILE:HG12 | 1.90 | 0.71 |
| 5:L:66:ILE:HD12 | 5:L:96:THR:CG2 | 2.20 | 0.71 |
| 11:A:829:G:N2 | 11:A:857:C:O2 | 2.14 | 0.71 |
| 1:D:33:ILE:HG22 | 1:D:34:GLU:N | 1.98 | 0.71 |
| 11:A:601:G:N2 | 11:A:637:C:O2 | 2.19 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 11:A:663:A:N6 | 11:A:742:G:H1 | 1.86 | 0.71 |
| 1:D:8:LEU:HD23 | 11:A:429:U:C5' | 2.20 | 0.70 |
| 11:A:454:G:H22 | 11:A:478:A:H2 | 1.36 | 0.70 |
| 11:A:1392:G:N2 | 11:A:1502:A:O5' | 2.24 | 0.70 |
| 11:A:748:G:H2' | 11:A:749:A:H8 | 1.56 | 0.70 |
| 6:O:53:ARG:NH1 | 11:A:579:A:O2' | 2.21 | 0.70 |
| 11:A:182:A:H2 | 11:A:194:C:H42 | 1.39 | 0.70 |
| 1:D:30:LYS:O | 1:D:31:CYS:SG | 2.48 | 0.70 |
| 11:A:457:G:N1 | 11:A:475:C:N3 | 2.33 | 0.70 |
| 4:K:28:ASN:OD1 | 4:K:46:ALA:HB3 | 1.92 | 0.70 |
| 5:L:113:ARG:NH2 | 11:A:501:C:OP1 | 2.24 | 0.70 |
| 11:A:86:G:H1' | 11:A:87:C:C5 | 2.27 | 0.70 |
| 11:A:94:G:N1 | 11:A:97:G:O6 | 2.24 | 0.70 |
| 11:A:697:U:O2' | 11:A:785:G:N3 | 2.24 | 0.69 |
| 11:A:859:G:OP2 | 11:A:869:G:N1 | 2.24 | 0.69 |
| 1:D:58:GLN:O | 1:D:62:ARG:HG2 | 1.92 | 0.69 |
| 2:F:10:VAL:O | 2:F:58:HIS:N | 2.25 | 0.69 |
| 3:H:61:THR:HG23 | 3:H:61:THR:O | 1.91 | 0.69 |
| 3:H:55:LYS:NZ | 11:A:652:U:O3' | 2.22 | 0.69 |
| 10:T:8:LYS:NZ | 10:T:12:GLN:OE1 | 2.26 | 0.69 |
| 1:D:9:LYS:CG | 1:D:37:PRO:HB2 | 2.22 | 0.69 |
| 8:Q:47:ASP:HA | 12:Q:103:HOH:O | 1.91 | 0.69 |
| 11:A:206:C:C6 | 12:A:1732:HOH:O | 2.45 | 0.69 |
| 4:K:46:ALA:HB2 | 4:K:65:ALA:HB2 | 1.74 | 0.69 |
| 7:P:71:VAL:O | 7:P:75:ILE:HG13 | 1.92 | 0.69 |
| 11:A:736:C:H2' | 11:A:737:C:C6 | 2.28 | 0.69 |
| 11:A:861:G:O6 | 11:A:869:G:N2 | 2.25 | 0.69 |
| 11:A:204:G:C4 | 11:A:465:A:H1' | 2.28 | 0.69 |
| 11:A:509:A:N3 | 11:A:543:U:O2' | 2.26 | 0.69 |
| 11:A:714:G:O2' | 11:A:777:A:N6 | 2.26 | 0.68 |
| 1:D:197:HIS:HA | 1:D:200:VAL:HG22 | 1.74 | 0.68 |
| 11:A:297:G:N2 | 11:A:300:A:OP2 | 2.19 | 0.68 |
| 11:A:744:C:H2' | 11:A:745:G:C8 | 2.28 | 0.68 |
| 11:A:674:G:N2 | 11:A:717:U:O2 | 2.26 | 0.68 |
| 11:A:693:G:H1 | 11:A:788:U:H4' | 1.58 | 0.68 |
| 4:K:62:ALA:HB1 | 4:K:95:THR:HB | 1.75 | 0.68 |
| 4:K:100:ASN:ND2 | 4:K:104:PHE:O | 2.26 | 0.68 |
| 11:A:837:U:O2 | 11:A:849:G:O6 | 2.12 | 0.68 |
| 11:A:204:G:C8 | 11:A:465:A:H8 | 2.12 | 0.68 |
| 1:D:56:GLU:HG2 | 1:D:198:LEU:HD13 | 1.74 | 0.68 |
| 11:A:465:A:H3' | 11:A:465:A:N3 | 2.09 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 4:K:28:ASN:ND2 | 11:A:689:C:OP1 | 2.27 | 0.67 |
| 7:P:18:GLN:OE1 | 7:P:35:ARG:NH1 | 2.24 | 0.67 |
| 11:A:159:G:N2 | 11:A:162:A:OP2 | 2.20 | 0.67 |
| 11:A:1507:A:H2' | 11:A:1508:A:C8 | 2.29 | 0.67 |
| 8:Q:27:PHE:CE2 | 8:Q:36:PHE:HB3 | 2.29 | 0.67 |
| 11:A:443:C:N3 | 11:A:491:G:N1 | 2.32 | 0.67 |
| 11:A:76:G:H3' | 11:A:77:A:H8 | 1.59 | 0.67 |
| 11:A:578:C:O2' | 11:A:728:A:N3 | 2.22 | 0.67 |
| 11:A:744:C:H2' | 11:A:745:G:H8 | 1.56 | 0.67 |
| 11:A:514:C:H3' | 11:A:532:A:H61 | 1.58 | 0.67 |
| 2:F:5:GLU:HA | 2:F:63:ASN:HA | 1.75 | 0.67 |
| 8:Q:30:HIS:N | 8:Q:35:LYS:O | 2.27 | 0.67 |
| 11:A:898:G:N2 | 11:A:901:A:OP2 | 2.28 | 0.67 |
| 11:A:1518:A:O2' | 11:A:1519:A:O5' | 2.13 | 0.67 |
| 1:D:187:ARG:O | 1:D:187:ARG:NH1 | 2.28 | 0.66 |
| 11:A:443:C:O2 | 11:A:491:G:N2 | 2.16 | 0.66 |
| 1:D:4:LEU:HD23 | 11:A:406:G:O5' | 1.93 | 0.66 |
| 11:A:522:C:H1' | 11:A:536:C:H5'' | 1.77 | 0.66 |
| 2:F:12:PRO:HG3 | 2:F:56:LYS:HB2 | 1.77 | 0.66 |
| 11:A:441:A:H61 | 11:A:493:A:N6 | 1.93 | 0.66 |
| 11:A:685:G:O2' | 11:A:686:U:O4' | 2.13 | 0.66 |
| 11:A:193:C:H5 | 12:A:1808:HOH:O | 1.77 | 0.66 |
| 11:A:455:G:C8 | 12:A:1652:HOH:O | 2.48 | 0.66 |
| 11:A:334:C:O2' | 11:A:335:C:H5' | 1.95 | 0.65 |
| 5:L:71:HIS:CD2 | 5:L:73:LEU:H | 2.14 | 0.65 |
| 11:A:8:A:O2' | 11:A:559:A:OP2 | 2.13 | 0.65 |
| 5:L:66:ILE:HD11 | 5:L:98:ARG:HH11 | 1.59 | 0.65 |
| 11:A:11:G:HO2' | 11:A:525:C:HO2' | 1.41 | 0.65 |
| 11:A:22:G:O2' | 11:A:913:A:N1 | 2.26 | 0.65 |
| 11:A:462:G:N2 | 11:A:470:C:O2 | 2.18 | 0.65 |
| 1:D:8:LEU:HD23 | 1:D:31:CYS:CB | 2.26 | 0.65 |
| 7:P:74:LEU:CD2 | 12:P:107:HOH:O | 2.44 | 0.65 |
| 4:K:80:ASN:HA | 4:K:105:ARG:H | 1.62 | 0.65 |
| 11:A:181:A:O2' | 11:A:194:C:N4 | 2.30 | 0.65 |
| 11:A:714:G:O2' | 11:A:715:A:O4' | 2.15 | 0.65 |
| 11:A:15:G:OP1 | 11:A:1397:C:N4 | 2.29 | 0.64 |
| 11:A:674:G:H2' | 11:A:675:A:C8 | 2.31 | 0.64 |
| 1:D:119:HIS:ND1 | 11:A:437:U:O2' | 2.23 | 0.64 |
| 2:F:37:HIS:HB2 | 2:F:97:THR:HG23 | 1.78 | 0.64 |
| 11:A:839:C:N4 | 11:A:847:G:O6 | 2.30 | 0.64 |
| 10:T:48:LYS:O | 10:T:52:GLU:HG2 | 1.97 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 11:A:837:U:H2' | 11:A:838:G:H8 | 1.61 | 0.64 |
| 11:A:459:A:P | 11:A:474:G:H22 | 2.21 | 0.64 |
| 11:A:926:G:OP2 | 11:A:927:G:N2 | 2.31 | 0.64 |
| 11:A:171:A:H2' | 11:A:172:A:C8 | 2.33 | 0.64 |
| 7:P:74:LEU:HD21 | 12:P:107:HOH:O | 1.98 | 0.64 |
| 11:A:727:G:N2 | 11:A:730:G:OP2 | 2.23 | 0.64 |
| 1:D:30:LYS:HE3 | 11:A:410:G:N7 | 2.12 | 0.63 |
| 9:R:41:SER:OG | 9:R:42:ARG:NH2 | 2.31 | 0.63 |
| 11:A:204:G:C5 | 11:A:465:A:H1' | 2.34 | 0.63 |
| 11:A:411:A:C6 | 11:A:430:A:N7 | 2.65 | 0.63 |
| 3:H:122:GLY:HA2 | 12:A:1774:HOH:O | 1.97 | 0.63 |
| 1:D:25:ARG:HD3 | 1:D:30:LYS:CD | 2.27 | 0.63 |
| 6:O:41:HIS:CD2 | 11:A:739:C:O2' | 2.51 | 0.63 |
| 11:A:747:A:H2' | 11:A:748:G:C8 | 2.34 | 0.63 |
| 1:D:68:GLU:OE1 | 1:D:72:ARG:NH2 | 2.32 | 0.63 |
| 11:A:407:U:H2' | 11:A:408:A:C8 | 2.33 | 0.63 |
| 11:A:444:G:O6 | 11:A:490:C:N4 | 2.28 | 0.63 |
| 4:K:52:ARG:NH1 | 11:A:690:G:N7 | 2.44 | 0.63 |
| 11:A:244:U:O4 | 11:A:893:C:N3 | 2.31 | 0.63 |
| 5:L:53:ARG:HG3 | 5:L:61:GLU:OE2 | 1.99 | 0.62 |
| 1:D:25:ARG:HD3 | 1:D:30:LYS:HD2 | 1.81 | 0.62 |
| 5:L:66:ILE:HD11 | 5:L:98:ARG:NH1 | 2.15 | 0.62 |
| 11:A:632:U:H5'' | 11:A:633:G:C8 | 2.35 | 0.62 |
| 1:D:69:ARG:NH2 | 11:A:401:C:OP2 | 2.33 | 0.62 |
| 11:A:59:A:H5'' | 11:A:387:U:H5'' | 1.81 | 0.62 |
| 1:D:9:LYS:CD | 1:D:37:PRO:HB2 | 2.30 | 0.62 |
| 2:F:42:TRP:O | 2:F:45:ARG:NH1 | 2.27 | 0.62 |
| 11:A:519:C:N4 | 11:A:529:G:O2' | 2.32 | 0.62 |
| 11:A:651:C:N4 | 11:A:753:A:OP2 | 2.32 | 0.62 |
| 11:A:84:U:H2' | 11:A:86:G:H21 | 1.63 | 0.62 |
| 11:A:352:C:O2' | 11:A:354:G:OP1 | 2.12 | 0.62 |
| 11:A:911:U:H2' | 11:A:912:C:C6 | 2.35 | 0.62 |
| 1:D:9:LYS:HG3 | 1:D:37:PRO:CG | 2.29 | 0.62 |
| 1:D:49:ASP:O | 1:D:53:GLN:HG3 | 1.99 | 0.62 |
| 5:L:19:ASN:OD1 | 5:L:20:VAL:N | 2.31 | 0.62 |
| 5:L:113:ARG:HG2 | 5:L:118:VAL:HG13 | 1.81 | 0.62 |
| 3:H:110:MET:HG2 | 3:H:114:ALA:HB3 | 1.82 | 0.61 |
| 11:A:675:A:H3' | 11:A:676:A:H8 | 1.66 | 0.61 |
| 4:K:16:SER:HA | 4:K:78:ILE:HA | 1.81 | 0.61 |
| 11:A:343:U:O2' | 11:A:346:G:O6 | 2.09 | 0.61 |
| 11:A:427:U:OP2 | 11:A:428:G:O2' | 2.16 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:F:14:GLN:HG2 | 2:F:83:ALA:HA | 1.80 | 0.61 |
| 4:K:33:ILE:O | 4:K:41:LEU:N | 2.23 | 0.61 |
| 4:K:51:PHE:HB2 | 4:K:55:ARG:HH22 | 1.65 | 0.61 |
| 5:L:106:VAL:HG23 | 5:L:109:ARG:HB2 | 1.81 | 0.61 |
| 6:O:64:LYS:NZ | 11:A:581:G:OP1 | 2.33 | 0.61 |
| 1:D:4:LEU:HD23 | 11:A:406:G:C5' | 2.30 | 0.61 |
| 1:D:75:TYR:HD1 | 1:D:89:LEU:CD1 | 2.13 | 0.61 |
| 6:O:22:GLY:HA3 | 11:A:750:C:O2 | 2.01 | 0.60 |
| 11:A:17:U:H2' | 11:A:18:C:H6 | 1.66 | 0.60 |
| 11:A:204:G:C8 | 11:A:465:A:C8 | 2.89 | 0.60 |
| 6:O:32:THR:HB | 6:O:62:ARG:HD2 | 1.83 | 0.60 |
| 11:A:411:A:N1 | 11:A:430:A:N7 | 2.48 | 0.60 |
| 9:R:31:TYR:HE1 | 9:R:44:THR:HG21 | 1.67 | 0.60 |
| 8:Q:25:GLU:OE2 | 8:Q:38:LYS:HB3 | 2.02 | 0.60 |
| 11:A:450:G:H5'' | 11:A:451:A:C5' | 2.32 | 0.60 |
| 11:A:908:A:H2' | 11:A:909:A:H8 | 1.67 | 0.60 |
| 1:D:10:LEU:HD21 | 1:D:62:ARG:HD2 | 1.83 | 0.60 |
| 2:F:11:HIS:O | 2:F:15:SER:N | 2.35 | 0.60 |
| 3:H:81:GLY:O | 3:H:82:LEU:HD22 | 2.01 | 0.60 |
| 11:A:89:U:H2' | 11:A:90:C:C6 | 2.37 | 0.59 |
| 11:A:207:C:C5 | 12:A:1732:HOH:O | 2.37 | 0.59 |
| 5:L:66:ILE:HD13 | 5:L:73:LEU:HD11 | 1.83 | 0.59 |
| 6:O:71:ARG:NH2 | 11:A:754:C:O5' | 2.35 | 0.59 |
| 8:Q:25:GLU:OE1 | 8:Q:40:THR:OG1 | 2.20 | 0.59 |
| 11:A:804:U:OP2 | 11:A:805:C:N4 | 2.33 | 0.59 |
| 11:A:842:U:O2' | 11:A:843:U:OP1 | 2.20 | 0.59 |
| 11:A:740:U:H2' | 11:A:741:G:C8 | 2.36 | 0.59 |
| 3:H:94:VAL:HG21 | 3:H:101:ALA:HB2 | 1.85 | 0.59 |
| 11:A:335:C:O2' | 11:A:336:A:H8 | 1.75 | 0.59 |
| 6:O:1:SER:OG | 11:A:740:U:OP1 | 2.21 | 0.59 |
| 6:O:6:ALA:HA | 6:O:9:LYS:HG2 | 1.85 | 0.59 |
| 11:A:266:G:O2' | 11:A:267:C:H3' | 2.03 | 0.59 |
| 11:A:91:U:H2' | 11:A:92:U:C6 | 2.38 | 0.58 |
| 11:A:919:A:H2' | 11:A:920:U:C6 | 2.38 | 0.58 |
| 11:A:925:G:O2' | 11:A:1503:A:N6 | 2.32 | 0.58 |
| 1:D:149:LYS:HB3 | 1:D:177:MET:CE | 2.33 | 0.58 |
| 5:L:66:ILE:HA | 5:L:96:THR:CG2 | 2.33 | 0.58 |
| 5:L:97:VAL:HG12 | 5:L:100:ALA:HB2 | 1.84 | 0.58 |
| 3:H:55:LYS:HZ1 | 11:A:653:U:P | 2.27 | 0.58 |
| 4:K:58:THR:HG23 | 4:K:61:ALA:H | 1.69 | 0.58 |
| 7:P:47:GLU:OE1 | 11:A:616:G:O2' | 2.21 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 11:A:79:G:O6 | 11:A:90:C:N4 | 2.24 | 0.58 |
| 11:A:465:A:H3' | 11:A:465:A:C4 | 2.39 | 0.58 |
| 11:A:789:U:C2 | 11:A:791:G:H5'' | 2.38 | 0.58 |
| 4:K:12:ARG:NH1 | 4:K:40:ALA:O | 2.34 | 0.58 |
| 11:A:76:G:O6 | 11:A:93:U:O4 | 2.20 | 0.58 |
| 11:A:493:A:H3' | 11:A:494:G:C8 | 2.37 | 0.58 |
| 3:H:38:VAL:O | 3:H:42:GLU:HG3 | 2.03 | 0.58 |
| 5:L:11:ARG:NH1 | 11:A:563:A:N3 | 2.51 | 0.58 |
| 10:T:56:ILE:O | 10:T:60:GLN:HG2 | 2.02 | 0.58 |
| 7:P:54:LEU:HD23 | 7:P:57:ILE:HD12 | 1.84 | 0.58 |
| 11:A:1520:C:H2' | 11:A:1521:C:C6 | 2.38 | 0.58 |
| 5:L:17:LYS:NZ | 11:A:885:G:O6 | 2.36 | 0.58 |
| 11:A:203:G:H1' | 11:A:465:A:N7 | 2.18 | 0.58 |
| 5:L:56:LEU:HD21 | 5:L:81:ILE:HD11 | 1.86 | 0.58 |
| 5:L:98:ARG:HH21 | 5:L:106:VAL:HG12 | 1.67 | 0.58 |
| 1:D:56:GLU:CD | 1:D:198:LEU:HB2 | 2.23 | 0.58 |
| 2:F:3:HIS:HB2 | 2:F:92:THR:HB | 1.85 | 0.58 |
| 2:F:10:VAL:HG11 | 2:F:18:VAL:HG22 | 1.86 | 0.58 |
| 11:A:435:A:C8 | 12:A:1632:HOH:O | 2.52 | 0.58 |
| 4:K:28:ASN:ND2 | 4:K:45:THR:OG1 | 2.35 | 0.58 |
| 11:A:747:A:H2' | 11:A:748:G:H8 | 1.68 | 0.58 |
| 2:F:26:THR:HG22 | 2:F:62:MET:CE | 2.34 | 0.57 |
| 11:A:908:A:H2' | 11:A:909:A:C8 | 2.39 | 0.57 |
| 11:A:121:U:H5'' | 12:A:1609:HOH:O | 2.02 | 0.57 |
| 11:A:252:U:O4 | 11:A:253:A:N6 | 2.38 | 0.57 |
| 11:A:462:G:P | 11:A:462:G:C8 | 2.98 | 0.57 |
| 11:A:695:A:H2' | 11:A:696:A:O4' | 2.04 | 0.57 |
| 11:A:715:A:OP1 | 11:A:805:C:O2' | 2.20 | 0.57 |
| 11:A:766:A:N7 | 11:A:813:U:O2 | 2.38 | 0.57 |
| 4:K:22:ILE:HA | 4:K:31:VAL:HG22 | 1.85 | 0.57 |
| 5:L:69:GLU:HG2 | 11:A:521:G:H4' | 1.87 | 0.57 |
| 11:A:487:A:H3' | 11:A:488:C:H6 | 1.70 | 0.57 |
| 11:A:788:U:H3' | 11:A:789:U:C6 | 2.40 | 0.57 |
| 2:F:8:PHE:HB2 | 2:F:84:VAL:HG11 | 1.85 | 0.57 |
| 7:P:76:LYS:HG2 | 7:P:80:LYS:HE3 | 1.87 | 0.57 |
| 11:A:779:C:O2' | 11:A:780:A:O4' | 2.20 | 0.57 |
| 1:D:32:LYS:O | 1:D:33:ILE:HD13 | 2.05 | 0.57 |
| 8:Q:16:MET:SD | 11:A:253:A:O2' | 2.61 | 0.57 |
| 11:A:12:U:O2 | 11:A:22:G:O6 | 2.23 | 0.57 |
| 11:A:157:U:H1' | 11:A:165:G:N2 | 2.20 | 0.57 |
| 11:A:832:G:N2 | 11:A:854:U:O2 | 2.32 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:F:36:ILE:HD13 | 2:F:62:MET:CE | 2.34 | 0.57 |
| 5:L:58:ASN:OD1 | 5:L:60:PHE:HD2 | 1.87 | 0.57 |
| 10:T:2:ASN:HD21 | 10:T:7:LYS:HG2 | 1.70 | 0.57 |
| 1:D:112:GLU:OE1 | 11:A:407:U:O2' | 2.23 | 0.56 |
| 1:D:56:GLU:HG2 | 1:D:198:LEU:HD12 | 1.87 | 0.56 |
| 6:O:77:TYR:O | 6:O:81:ILE:HG12 | 2.04 | 0.56 |
| 11:A:79:G:H2' | 11:A:80:A:C8 | 2.40 | 0.56 |
| 11:A:450:G:H5' | 11:A:451:A:H5' | 1.88 | 0.56 |
| 11:A:487:A:H3' | 11:A:488:C:C6 | 2.41 | 0.56 |
| 11:A:670:G:C6 | 11:A:671:G:O6 | 2.58 | 0.56 |
| 11:A:767:A:O2' | 11:A:1524:C:O2 | 2.24 | 0.56 |
| 11:A:693:G:N1 | 11:A:788:U:H4' | 2.21 | 0.56 |
| 5:L:56:LEU:HD21 | 5:L:81:ILE:CD1 | 2.36 | 0.56 |
| 9:R:33:THR:HG22 | 9:R:37:LYS:H | 1.71 | 0.56 |
| 11:A:721:G:H5' | 11:A:722:G:C8 | 2.41 | 0.56 |
| 11:A:1501:C:OP2 | 11:A:1504:G:O2' | 2.23 | 0.56 |
| 11:A:126:G:OP1 | 11:A:605:U:O2' | 2.19 | 0.56 |
| 11:A:335:C:O2' | 11:A:336:A:O5' | 2.23 | 0.56 |
| 2:F:44:ARG:HG2 | 2:F:56:LYS:HB3 | 1.87 | 0.56 |
| 11:A:464:U:H2' | 11:A:466:A:OP1 | 2.06 | 0.56 |
| 11:A:847:G:H2' | 11:A:848:C:C6 | 2.41 | 0.56 |
| 9:R:36:GLY:O | 9:R:62:ARG:NH2 | 2.39 | 0.56 |
| 11:A:21:G:H2' | 11:A:22:G:C8 | 2.40 | 0.56 |
| 2:F:2:ARG:HD3 | 2:F:92:THR:HG23 | 1.86 | 0.55 |
| 9:R:22:TYR:HA | 9:R:57:ALA:HB1 | 1.88 | 0.55 |
| 11:A:269:C:H2' | 11:A:270:A:C8 | 2.42 | 0.55 |
| 11:A:382:A:H2' | 11:A:383:A:C8 | 2.41 | 0.55 |
| 11:A:692:U:N3 | 11:A:695:A:OP2 | 2.28 | 0.55 |
| 11:A:1508:A:H2' | 11:A:1509:C:O4' | 2.06 | 0.55 |
| 2:F:18:VAL:HG13 | 2:F:22:ILE:HD11 | 1.88 | 0.55 |
| 5:L:33:CYS:H | 5:L:54:VAL:HG23 | 1.70 | 0.55 |
| 3:H:39:LEU:O | 3:H:43:GLY:N | 2.37 | 0.55 |
| 5:L:98:ARG:HH21 | 5:L:106:VAL:CG1 | 2.19 | 0.55 |
| 6:O:4:THR:O | 6:O:7:THR:OG1 | 2.21 | 0.55 |
| 6:O:32:THR:HG21 | 6:O:84:LEU:HD21 | 1.88 | 0.55 |
| 7:P:7:ALA:HB1 | 7:P:29:ASN:HB3 | 1.88 | 0.55 |
| 11:A:90:C:H2' | 11:A:91:U:C6 | 2.41 | 0.55 |
| 11:A:691:G:H1' | 11:A:696:A:N6 | 2.21 | 0.55 |
| 11:A:1526:G:H2' | 11:A:1527:U:C6 | 2.41 | 0.55 |
| 1:D:4:LEU:HD23 | 11:A:406:G:H5' | 1.88 | 0.55 |
| 1:D:171:GLU:HG3 | 1:D:182:LYS:HD2 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 4:K:12:ARG:NH1 | 11:A:684:U:O3' | 2.39 | 0.55 |
| 6:O:35:ILE:HD12 | 6:O:62:ARG:CZ | 2.36 | 0.55 |
| 1:D:150:LYS:HD2 | 1:D:150:LYS:O | 2.07 | 0.55 |
| 3:H:12:ARG:NH1 | 11:A:826:C:C5' | 2.69 | 0.55 |
| 11:A:410:G:C6 | 11:A:429:U:O2' | 2.58 | 0.55 |
| 11:A:782:A:H3' | 11:A:783:C:H6 | 1.71 | 0.55 |
| 11:A:362:G:N1 | 11:A:365:U:OP2 | 2.37 | 0.55 |
| 1:D:8:LEU:CD2 | 11:A:429:U:H5' | 2.34 | 0.55 |
| 5:L:55:ARG:HB2 | 5:L:61:GLU:OE1 | 2.06 | 0.55 |
| 5:L:113:ARG:CG | 5:L:118:VAL:HG13 | 2.36 | 0.55 |
| 11:A:740:U:H2' | 11:A:741:G:H8 | 1.71 | 0.55 |
| 1:D:104:MET:HG2 | 1:D:170:LEU:HD13 | 1.89 | 0.55 |
| 11:A:448:A:H5'' | 12:A:1666:HOH:O | 2.07 | 0.55 |
| 11:A:837:U:H2' | 11:A:838:G:C8 | 2.41 | 0.55 |
| 1:D:109:THR:H | 1:D:112:GLU:HB3 | 1.72 | 0.55 |
| 8:Q:8:GLN:NE2 | 8:Q:78:VAL:HG21 | 2.22 | 0.55 |
| 11:A:31:G:HO2' | 11:A:48:C:N4 | 2.05 | 0.55 |
| 11:A:1525:G:H2' | 11:A:1526:G:H8 | 1.70 | 0.55 |
| 6:O:47:LYS:CE | 11:A:808:C:OP1 | 2.46 | 0.54 |
| 11:A:147:G:H2' | 11:A:148:G:C8 | 2.42 | 0.54 |
| 1:D:60:VAL:HG21 | 1:D:199:ILE:HD11 | 1.89 | 0.54 |
| 6:O:27:GLN:O | 6:O:31:LEU:HG | 2.07 | 0.54 |
| 11:A:459:A:H2' | 11:A:460:A:H8 | 1.72 | 0.54 |
| 1:D:137:SER:OG | 1:D:140:ASP:OD2 | 2.23 | 0.54 |
| 2:F:38:ARG:HG2 | 2:F:63:ASN:HB2 | 1.89 | 0.54 |
| 7:P:14:ARG:HA | 7:P:42:ILE:CD1 | 2.36 | 0.54 |
| 11:A:131:A:H2' | 11:A:132:C:C6 | 2.42 | 0.54 |
| 1:D:4:LEU:HD21 | 11:A:406:G:O5' | 2.06 | 0.54 |
| 11:A:70:U:O2' | 11:A:94:G:N7 | 2.38 | 0.54 |
| 11:A:601:G:H2' | 11:A:602:A:C8 | 2.43 | 0.54 |
| 11:A:658:C:N4 | 11:A:748:G:O6 | 2.41 | 0.54 |
| 11:A:768:A:H4' | 11:A:1523:G:N2 | 2.21 | 0.54 |
| 8:Q:42:LYS:NZ | 11:A:278:G:OP2 | 2.35 | 0.54 |
| 11:A:62:U:H2' | 11:A:63:C:C6 | 2.43 | 0.54 |
| 11:A:475:C:H2' | 11:A:476:U:C6 | 2.41 | 0.54 |
| 2:F:9:MET:HB2 | 2:F:57:ALA:HB1 | 1.88 | 0.54 |
| 11:A:11:G:O2' | 11:A:525:C:O2' | 2.17 | 0.54 |
| 8:Q:69:THR:OG1 | 11:A:254:G:OP1 | 2.24 | 0.54 |
| 11:A:779:C:H2' | 11:A:780:A:C5 | 2.43 | 0.54 |
| 6:O:80:LEU:HA | 6:O:83:ARG:HG2 | 1.90 | 0.54 |
| 11:A:462:G:P | 11:A:462:G:H8 | 2.30 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 11:A:840:C:H2' | 11:A:841:C:H5'' | 1.90 | 0.54 |
| 10:T:2:ASN:HA | 11:A:332:G:OP2 | 2.07 | 0.54 |
| 11:A:737:C:H2' | 11:A:738:C:H6 | 1.71 | 0.54 |
| 7:P:14:ARG:HA | 7:P:42:ILE:HD13 | 1.90 | 0.54 |
| 11:A:374:A:H5'' | 11:A:452:A:C2 | 2.43 | 0.54 |
| 11:A:710:G:H2' | 11:A:711:G:C8 | 2.43 | 0.54 |
| 1:D:33:ILE:CG2 | 1:D:34:GLU:H | 2.00 | 0.53 |
| 3:H:79:ARG:HD2 | 11:A:878:A:OP1 | 2.09 | 0.53 |
| 1:D:97:LEU:HA | 1:D:100:VAL:HG12 | 1.89 | 0.53 |
| 4:K:33:ILE:HD12 | 4:K:81:LEU:HD13 | 1.89 | 0.53 |
| 6:O:32:THR:HB | 6:O:86:LEU:HD11 | 1.89 | 0.53 |
| 10:T:58:ASP:OD2 | 11:A:194:C:O4' | 2.25 | 0.53 |
| 10:T:43:LYS:HD3 | 10:T:86:ALA:HA | 1.91 | 0.53 |
| 11:A:251:G:C6 | 11:A:266:G:C2 | 2.96 | 0.53 |
| 4:K:52:ARG:HB3 | 11:A:691:G:O6 | 2.08 | 0.53 |
| 5:L:18:SER:HB3 | 5:L:21:PRO:HB3 | 1.90 | 0.53 |
| 11:A:779:C:H2' | 11:A:780:A:C4 | 2.44 | 0.53 |
| 11:A:1525:G:H2' | 11:A:1526:G:C8 | 2.43 | 0.53 |
| 1:D:4:LEU:CD2 | 11:A:406:G:C5' | 2.86 | 0.53 |
| 11:A:266:G:O2' | 11:A:267:C:O5' | 2.25 | 0.53 |
| 11:A:730:G:O2' | 11:A:814:A:N6 | 2.42 | 0.53 |
| 11:A:735:C:H2' | 11:A:736:C:C6 | 2.44 | 0.53 |
| 11:A:838:G:H2' | 11:A:839:C:H6 | 1.73 | 0.53 |
| 1:D:33:ILE:HB | 1:D:34:GLU:OE1 | 2.08 | 0.53 |
| 2:F:46:GLN:HE22 | 2:F:56:LYS:HG3 | 1.74 | 0.53 |
| 3:H:1:SER:H2 | 3:H:5:PRO:HA | 1.74 | 0.53 |
| 3:H:42:GLU:OE2 | 3:H:44:PHE:CD2 | 2.46 | 0.53 |
| 4:K:32:THR:HB | 11:A:705:G:H22 | 1.73 | 0.53 |
| 11:A:18:C:H2' | 11:A:19:A:O4' | 2.09 | 0.53 |
| 11:A:665:A:H2' | 11:A:732:C:O2 | 2.09 | 0.53 |
| 3:H:12:ARG:HH12 | 11:A:826:C:H5'' | 1.74 | 0.53 |
| 6:O:47:LYS:HE2 | 11:A:808:C:P | 2.49 | 0.52 |
| 11:A:500:G:H2' | 11:A:501:C:C6 | 2.44 | 0.52 |
| 11:A:843:U:H4' | 11:A:844:G:OP1 | 2.09 | 0.52 |
| 8:Q:57:VAL:O | 8:Q:78:VAL:HG22 | 2.09 | 0.52 |
| 11:A:371:A:H2' | 11:A:372:C:O4' | 2.08 | 0.52 |
| 11:A:575:G:H4' | 11:A:576:C:H5'' | 1.91 | 0.52 |
| 11:A:592:G:C6 | 11:A:648:A:C6 | 2.97 | 0.52 |
| 11:A:658:C:C2 | 11:A:748:G:N2 | 2.77 | 0.52 |
| 11:A:681:A:N6 | 11:A:682:G:O6 | 2.41 | 0.52 |
| 11:A:734:G:H2' | 11:A:735:C:C6 | 2.44 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 11:A:783:C:H2' | 11:A:784:A:C8 | 2.44 | 0.52 |
| 11:A:925:G:H1' | 11:A:1392:G:O6 | 2.08 | 0.52 |
| 2:F:4:TYR:CD2 | 2:F:66:ALA:HB3 | 2.44 | 0.52 |
| 11:A:204:G:C4 | 11:A:205:A:C8 | 2.98 | 0.52 |
| 11:A:832:G:H2' | 11:A:833:G:C8 | 2.45 | 0.52 |
| 5:L:71:HIS:HD2 | 5:L:73:LEU:H | 1.54 | 0.52 |
| 9:R:49:LYS:HA | 9:R:52:ARG:HE | 1.73 | 0.52 |
| 6:O:45:HIS:C | 6:O:47:LYS:H | 2.13 | 0.52 |
| 10:T:77:ASN:O | 10:T:81:GLN:HG2 | 2.10 | 0.52 |
| 11:A:691:G:N2 | 11:A:696:A:C8 | 2.78 | 0.52 |
| 11:A:212:G:C4 | 11:A:213:G:C8 | 2.97 | 0.52 |
| 11:A:516:U:H3' | 11:A:517:G:C8 | 2.45 | 0.52 |
| 6:O:76:ARG:HG2 | 6:O:79:ARG:HH22 | 1.75 | 0.52 |
| 11:A:91:U:H2' | 11:A:92:U:H6 | 1.75 | 0.52 |
| 11:A:411:A:N1 | 11:A:430:A:C6 | 2.76 | 0.52 |
| 11:A:710:G:H2' | 11:A:711:G:H8 | 1.74 | 0.52 |
| 3:H:47:ASP:H | 3:H:61:THR:CG2 | 2.23 | 0.52 |
| 7:P:4:ILE:HD12 | 7:P:21:VAL:HG22 | 1.92 | 0.52 |
| 7:P:5:ARG:NH2 | 7:P:24:SER:O | 2.43 | 0.52 |
| 11:A:77:A:H2' | 11:A:78:A:O4' | 2.10 | 0.52 |
| 11:A:82:G:N2 | 11:A:84:U:O4 | 2.43 | 0.52 |
| 11:A:134:G:H1' | 11:A:325:A:C5 | 2.45 | 0.52 |
| 11:A:182:A:H1' | 11:A:183:C:C5 | 2.45 | 0.52 |
| 11:A:859:G:H2' | 11:A:860:A:C8 | 2.45 | 0.52 |
| 11:A:118:U:H3' | 11:A:288:A:H61 | 1.75 | 0.51 |
| 11:A:893:C:H2' | 11:A:894:G:C8 | 2.45 | 0.51 |
| 11:A:920:U:H2' | 11:A:921:U:C5 | 2.45 | 0.51 |
| 11:A:1393:U:H3' | 11:A:1394:A:C8 | 2.45 | 0.51 |
| 1:D:75:TYR:CD1 | 1:D:89:LEU:HD12 | 2.45 | 0.51 |
| 2:F:29:ILE:HD13 | 2:F:64:VAL:HG11 | 1.93 | 0.51 |
| 8:Q:13:SER:HA | 8:Q:54:ILE:CD1 | 2.40 | 0.51 |
| 11:A:1394:A:H2' | 11:A:1395:C:O4' | 2.10 | 0.51 |
| 2:F:37:HIS:ND1 | 2:F:65:GLU:HG3 | 2.25 | 0.51 |
| 5:L:97:VAL:CG1 | 5:L:100:ALA:HB2 | 2.40 | 0.51 |
| 9:R:42:ARG:NH1 | 11:A:721:G:OP2 | 2.42 | 0.51 |
| 11:A:150:U:H2' | 11:A:151:A:C8 | 2.46 | 0.51 |
| 11:A:737:C:H2' | 11:A:738:C:C6 | 2.46 | 0.51 |
| 5:L:66:ILE:HA | 5:L:96:THR:HG22 | 1.92 | 0.51 |
| 9:R:62:ARG:NH2 | 11:A:719:C:O2 | 2.38 | 0.51 |
| 11:A:658:C:H2' | 11:A:659:U:H6 | 1.75 | 0.51 |
| 11:A:770:C:H2' | 11:A:771:G:C8 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 11:A:785:G:H8 | 11:A:785:G:P | 2.34 | 0.51 |
| 2:F:38:ARG:NH1 | 2:F:98:GLU:O | 2.44 | 0.51 |
| 3:H:61:THR:O | 3:H:61:THR:CG2 | 2.58 | 0.51 |
| 11:A:675:A:H3' | 11:A:676:A:C8 | 2.44 | 0.51 |
| 3:H:21:LYS:O | 3:H:64:TYR:OH | 2.27 | 0.51 |
| 9:R:60:ARG:O | 9:R:64:LEU:N | 2.44 | 0.51 |
| 9:R:63:TYR:OH | 11:A:734:G:N3 | 2.39 | 0.51 |
| 10:T:61:ALA:HA | 10:T:66:ILE:O | 2.11 | 0.51 |
| 11:A:465:A:H4' | 11:A:466:A:N6 | 2.25 | 0.51 |
| 11:A:481:G:O2' | 11:A:483:C:N4 | 2.40 | 0.51 |
| 11:A:770:C:H2' | 11:A:771:G:H8 | 1.76 | 0.51 |
| 1:D:87:GLU:OE1 | 1:D:187:ARG:HB2 | 2.11 | 0.51 |
| 11:A:207:C:H2' | 11:A:208:U:O4' | 2.11 | 0.51 |
| 4:K:32:THR:HB | 11:A:705:G:N2 | 2.26 | 0.51 |
| 7:P:52:LEU:HD12 | 7:P:78:VAL:HG21 | 1.93 | 0.51 |
| 11:A:580:C:H2' | 11:A:581:G:O4' | 2.10 | 0.51 |
| 1:D:151:GLN:HE22 | 1:D:153:ARG:HE | 1.59 | 0.51 |
| 2:F:44:ARG:HA | 2:F:58:HIS:HA | 1.93 | 0.51 |
| 2:F:86:ARG:HG2 | 2:F:88:MET:SD | 2.51 | 0.51 |
| 3:H:39:LEU:HD21 | 3:H:128:VAL:HG21 | 1.92 | 0.50 |
| 4:K:105:ARG:NH1 | 4:K:106:ILE:O | 2.43 | 0.50 |
| 7:P:40:ASN:HB3 | 7:P:43:ALA:HB2 | 1.93 | 0.50 |
| 11:A:468:A:H5' | 11:A:469:C:OP2 | 2.11 | 0.50 |
| 11:A:728:A:H2' | 11:A:729:A:C8 | 2.46 | 0.50 |
| 1:D:75:TYR:HD1 | 1:D:89:LEU:HD12 | 1.74 | 0.50 |
| 3:H:10:LEU:HD22 | 3:H:74:ILE:HD11 | 1.93 | 0.50 |
| 9:R:48:ALA:O | 9:R:52:ARG:NE | 2.44 | 0.50 |
| 1:D:1:ALA:HB2 | 11:A:547:A:OP2 | 2.09 | 0.50 |
| 1:D:13:ARG:HH11 | 1:D:37:PRO:HD2 | 1.77 | 0.50 |
| 3:H:47:ASP:H | 3:H:61:THR:HG22 | 1.75 | 0.50 |
| 11:A:251:G:C4 | 11:A:266:G:C5 | 2.99 | 0.50 |
| 11:A:413:G:H4' | 11:A:414:A:H5'' | 1.93 | 0.50 |
| 11:A:836:G:O6 | 11:A:850:U:O4 | 2.29 | 0.50 |
| 2:F:36:ILE:HG21 | 2:F:62:MET:HE3 | 1.94 | 0.50 |
| 4:K:48:GLY:N | 4:K:52:ARG:HD3 | 2.26 | 0.50 |
| 5:L:22:ALA:HB3 | 5:L:94:TYR:OH | 2.11 | 0.50 |
| 11:A:722:G:H1 | 11:A:733:G:H1 | 1.59 | 0.50 |
| 1:D:75:TYR:OH | 1:D:200:VAL:HA | 2.11 | 0.50 |
| 8:Q:19:SER:HB3 | 8:Q:70:LYS:NZ | 2.26 | 0.50 |
| 11:A:429:U:H1' | 11:A:430:A:H5'' | 1.94 | 0.50 |
| 11:A:625:U:H2' | 11:A:626:G:C8 | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 11:A:785:G:H2' | 11:A:786:G:C8 | 2.47 | 0.50 |
| 5:L:46:SER:HB3 | 11:A:519:C:OP2 | 2.11 | 0.50 |
| 11:A:157:U:O2 | 11:A:164:G:C6 | 2.64 | 0.50 |
| 11:A:381:C:H2' | 11:A:382:A:O4' | 2.12 | 0.50 |
| 11:A:863:U:O2' | 11:A:865:A:N7 | 2.35 | 0.50 |
| 11:A:1393:U:H3' | 11:A:1394:A:H8 | 1.77 | 0.50 |
| 1:D:9:LYS:CG | 1:D:37:PRO:CB | 2.71 | 0.50 |
| 1:D:12:ARG:NH2 | 11:A:427:U:OP1 | 2.45 | 0.50 |
| 3:H:55:LYS:O | 3:H:57:GLU:OE1 | 2.30 | 0.50 |
| 8:Q:27:PHE:CZ | 8:Q:36:PHE:CB | 2.95 | 0.50 |
| 2:F:26:THR:HG22 | 2:F:62:MET:HE2 | 1.92 | 0.49 |
| 11:A:251:G:C4 | 11:A:266:G:C6 | 3.00 | 0.49 |
| 11:A:1513:A:H2' | 11:A:1514:G:H8 | 1.77 | 0.49 |
| 1:D:2:ARG:NH2 | 11:A:406:G:O3' | 2.40 | 0.49 |
| 3:H:103:VAL:HG23 | 3:H:105:THR:HG23 | 1.94 | 0.49 |
| 6:O:32:THR:CB | 6:O:86:LEU:HD11 | 2.43 | 0.49 |
| 9:R:46:THR:O | 9:R:46:THR:HG22 | 2.12 | 0.49 |
| 11:A:1520:C:H2' | 11:A:1521:C:H6 | 1.75 | 0.49 |
| 1:D:49:ASP:OD1 | 1:D:50:TYR:N | 2.45 | 0.49 |
| 3:H:2:MET:HE1 | 11:A:756:C:O4' | 2.11 | 0.49 |
| 1:D:109:THR:HG23 | 1:D:112:GLU:H | 1.77 | 0.49 |
| 1:D:160:LEU:HA | 1:D:163:GLN:OE1 | 2.12 | 0.49 |
| 8:Q:15:LYS:HE2 | 11:A:275:G:H5' | 1.94 | 0.49 |
| 10:T:27:MET:HG3 | 10:T:57:VAL:HG12 | 1.94 | 0.49 |
| 11:A:218:U:H2' | 11:A:219:U:O4' | 2.11 | 0.49 |
| 11:A:695:A:H61 | 11:A:786:G:N2 | 2.02 | 0.49 |
| 2:F:5:GLU:OE1 | 9:R:22:TYR:OH | 2.29 | 0.49 |
| 3:H:115:ALA:O | 3:H:119:GLY:N | 2.43 | 0.49 |
| 10:T:28:ARG:HG3 | 10:T:28:ARG:HH11 | 1.78 | 0.49 |
| 11:A:916:U:H2' | 11:A:917:G:H8 | 1.77 | 0.49 |
| 1:D:106:PHE:CD1 | 1:D:144:ILE:HD11 | 2.48 | 0.49 |
| 6:O:32:THR:HB | 6:O:62:ARG:CD | 2.42 | 0.49 |
| 11:A:711:G:H2' | 11:A:712:A:C8 | 2.47 | 0.49 |
| 1:D:149:LYS:CB | 1:D:177:MET:CE | 2.90 | 0.49 |
| 5:L:55:ARG:HG2 | 5:L:55:ARG:HH11 | 1.78 | 0.49 |
| 7:P:35:ARG:HD3 | 12:A:1924:HOH:O | 2.12 | 0.49 |
| 11:A:714:G:H21 | 11:A:777:A:H1' | 1.78 | 0.49 |
| 6:O:34:GLN:O | 6:O:38:LEU:HD13 | 2.13 | 0.49 |
| 6:O:35:ILE:HD12 | 6:O:62:ARG:NH1 | 2.28 | 0.49 |
| 6:O:38:LEU:CD2 | 6:O:55:LEU:CB | 2.89 | 0.49 |
| 11:A:505:G:H2' | 11:A:506:G:C8 | 2.48 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 11:A:517:G:O2' | 11:A:530:G:H4' | 2.13 | 0.49 |
| 11:A:713:G:O2' | 11:A:714:G:O4' | 2.13 | 0.49 |
| 1:D:8:LEU:CD2 | 11:A:429:U:C3' | 2.66 | 0.49 |
| 3:H:14:ARG:NH2 | 3:H:74:ILE:O | 2.43 | 0.49 |
| 1:D:104:MET:O | 1:D:172:VAL:HG21 | 2.13 | 0.49 |
| 7:P:4:ILE:CD1 | 7:P:21:VAL:HG22 | 2.42 | 0.49 |
| 2:F:4:TYR:HE1 | 2:F:91:ARG:HD3 | 1.76 | 0.48 |
| 10:T:3:ILE:N | 11:A:332:G:OP2 | 2.38 | 0.48 |
| 11:A:76:G:H3' | 11:A:77:A:C8 | 2.45 | 0.48 |
| 11:A:320:A:H2' | 11:A:321:A:O4' | 2.13 | 0.48 |
| 11:A:720:C:OP2 | 11:A:721:G:O2' | 2.30 | 0.48 |
| 11:A:735:C:H2' | 11:A:736:C:H6 | 1.78 | 0.48 |
| 11:A:745:G:H2' | 11:A:746:A:H8 | 1.78 | 0.48 |
| 11:A:768:A:H5' | 11:A:1524:C:H1' | 1.94 | 0.48 |
| 11:A:883:C:O2' | 11:A:884:U:H5' | 2.13 | 0.48 |
| 5:L:34:THR:O | 5:L:75:GLU:OE1 | 2.31 | 0.48 |
| 11:A:193:C:H2' | 11:A:194:C:C6 | 2.49 | 0.48 |
| 11:A:568:G:O2' | 11:A:574:A:N1 | 2.31 | 0.48 |
| 11:A:712:A:H3' | 11:A:713:G:C5 | 2.48 | 0.48 |
| 11:A:820:U:H4' | 11:A:821:G:OP2 | 2.13 | 0.48 |
| 11:A:838:G:H2' | 11:A:839:C:C6 | 2.47 | 0.48 |
| 11:A:863:U:H2' | 11:A:865:A:OP2 | 2.13 | 0.48 |
| 11:A:911:U:H2' | 11:A:912:C:H6 | 1.78 | 0.48 |
| 11:A:235:C:H2' | 11:A:236:A:C8 | 2.48 | 0.48 |
| 11:A:236:A:H2' | 11:A:237:G:C8 | 2.48 | 0.48 |
| 11:A:355:C:H2' | 11:A:356:A:O4' | 2.14 | 0.48 |
| 11:A:652:U:O4 | 11:A:752:G:O2' | 2.23 | 0.48 |
| 11:A:845:A:H2' | 11:A:846:G:H5' | 1.95 | 0.48 |
| 4:K:80:ASN:HB3 | 4:K:105:ARG:HE | 1.78 | 0.48 |
| 5:L:75:GLU:OE2 | 5:L:76:HIS:CE1 | 2.66 | 0.48 |
| 11:A:464:U:HO2' | 11:A:465:A:H2 | 1.59 | 0.48 |
| 11:A:670:G:C6 | 11:A:671:G:C6 | 3.02 | 0.48 |
| 11:A:840:C:N3 | 11:A:847:G:N1 | 2.61 | 0.48 |
| 11:A:1521:C:H2' | 11:A:1522:U:C6 | 2.48 | 0.48 |
| 2:F:7:VAL:HG22 | 2:F:61:LEU:HB2 | 1.96 | 0.48 |
| 3:H:94:VAL:CG2 | 3:H:101:ALA:HB2 | 2.43 | 0.48 |
| 4:K:12:ARG:NH1 | 11:A:684:U:O2' | 2.47 | 0.48 |
| 4:K:66:ALA:HB3 | 4:K:98:ALA:HB3 | 1.94 | 0.48 |
| 5:L:22:ALA:HB3 | 5:L:94:TYR:CZ | 2.49 | 0.48 |
| 9:R:38:ILE:HD12 | 11:A:720:C:H1' | 1.95 | 0.48 |
| 10:T:23:ARG:NH2 | 11:A:176:C:H5'' | 2.28 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 11:A:67:C:H2' | 11:A:68:G:C8 | 2.49 | 0.48 |
| 11:A:184:G:H2' | 11:A:185:U:C6 | 2.49 | 0.48 |
| 11:A:204:G:H2' | 11:A:205:A:O4' | 2.13 | 0.48 |
| 11:A:284:C:H2' | 11:A:285:C:C6 | 2.49 | 0.48 |
| 11:A:665:A:N7 | 11:A:724:G:C6 | 2.82 | 0.48 |
| 1:D:1:ALA:HB2 | 11:A:547:A:O5' | 2.14 | 0.48 |
| 2:F:20:GLY:O | 2:F:24:ARG:CG | 2.49 | 0.48 |
| 11:A:450:G:H5'' | 11:A:451:A:H5'' | 1.95 | 0.48 |
| 11:A:502:A:H2' | 11:A:503:C:O4' | 2.14 | 0.48 |
| 11:A:854:U:H2' | 11:A:855:U:H6 | 1.78 | 0.48 |
| 6:O:35:ILE:O | 6:O:39:GLN:HG2 | 2.14 | 0.48 |
| 11:A:361:G:H2' | 11:A:362:G:O4' | 2.14 | 0.48 |
| 11:A:539:A:H2' | 11:A:540:G:C8 | 2.48 | 0.48 |
| 11:A:678:U:H3 | 11:A:713:G:H22 | 1.61 | 0.48 |
| 11:A:778:G:H2' | 11:A:779:C:C6 | 2.49 | 0.48 |
| 3:H:110:MET:HG2 | 3:H:114:ALA:HB1 | 1.95 | 0.48 |
| 11:A:431:A:H2' | 11:A:432:A:O4' | 2.14 | 0.48 |
| 11:A:458:U:H2' | 11:A:474:G:C2 | 2.49 | 0.48 |
| 6:O:35:ILE:HD11 | 6:O:59:VAL:HA | 1.95 | 0.47 |
| 8:Q:6:THR:HA | 8:Q:60:ILE:O | 2.14 | 0.47 |
| 11:A:417:G:H2' | 11:A:418:C:C6 | 2.48 | 0.47 |
| 11:A:829:G:C6 | 11:A:858:G:C2 | 3.01 | 0.47 |
| 3:H:12:ARG:HH12 | 11:A:826:C:C5' | 2.26 | 0.47 |
| 3:H:17:GLN:HG2 | 3:H:62:LEU:HD13 | 1.96 | 0.47 |
| 11:A:114:U:H1' | 11:A:353:A:H1' | 1.95 | 0.47 |
| 11:A:121:U:C5' | 12:A:1609:HOH:O | 2.60 | 0.47 |
| 11:A:206:C:H2' | 11:A:207:C:H6 | 1.79 | 0.47 |
| 11:A:303:A:H2' | 11:A:304:U:O4' | 2.14 | 0.47 |
| 2:F:3:HIS:HA | 2:F:65:GLU:HG2 | 1.95 | 0.47 |
| 3:H:31:LEU:O | 3:H:35:ILE:HD12 | 2.13 | 0.47 |
| 4:K:31:VAL:HB | 4:K:69:CYS:SG | 2.54 | 0.47 |
| 11:A:830:G:H2' | 11:A:831:A:C8 | 2.49 | 0.47 |
| 2:F:26:THR:CG2 | 2:F:62:MET:HE1 | 2.45 | 0.47 |
| 5:L:66:ILE:HA | 5:L:96:THR:HG21 | 1.96 | 0.47 |
| 7:P:67:ILE:HG22 | 7:P:71:VAL:HB | 1.94 | 0.47 |
| 1:D:16:THR:OG1 | 1:D:17:ASP:N | 2.48 | 0.47 |
| 1:D:100:VAL:HG11 | 1:D:136:VAL:HG21 | 1.95 | 0.47 |
| 4:K:70:ALA:O | 4:K:74:LYS:HG2 | 2.14 | 0.47 |
| 8:Q:59:GLU:OE2 | 8:Q:76:ARG:NH2 | 2.48 | 0.47 |
| 11:A:419:C:H5 | 12:A:1701:HOH:O | 1.97 | 0.47 |
| 11:A:666:G:O4' | 11:A:726:C:O2' | 2.32 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:60:VAL:HG22 | 1:D:194:ILE:HD12 | 1.96 | 0.47 |
| 2:F:38:ARG:HH22 | 2:F:96:VAL:HG12 | 1.78 | 0.47 |
| 11:A:206:C:C5 | 12:A:1732:HOH:O | 2.66 | 0.47 |
| 11:A:213:G:C8 | 11:A:214:C:C5 | 3.02 | 0.47 |
| 11:A:486:U:H2' | 11:A:487:A:C8 | 2.49 | 0.47 |
| 3:H:57:GLU:OE1 | 3:H:57:GLU:N | 2.48 | 0.47 |
| 4:K:21:HIS:HB3 | 4:K:32:THR:HG22 | 1.96 | 0.47 |
| 5:L:87:LYS:HE3 | 11:A:523:A:H2 | 1.80 | 0.47 |
| 7:P:8:ARG:HH21 | 7:P:15:PRO:HG3 | 1.80 | 0.47 |
| 11:A:685:G:N2 | 11:A:706:A:N6 | 2.63 | 0.47 |
| 11:A:713:G:H2' | 11:A:714:G:C4 | 2.50 | 0.47 |
| 11:A:789:U:N3 | 11:A:792:A:OP2 | 2.29 | 0.47 |
| 3:H:1:SER:N | 3:H:8:ASP:HB2 | 2.30 | 0.47 |
| 8:Q:67:SER:OG | 8:Q:70:LYS:HB3 | 2.14 | 0.47 |
| 11:A:76:G:C6 | 11:A:77:A:C6 | 3.03 | 0.47 |
| 11:A:714:G:HO2' | 11:A:715:A:C1' | 2.27 | 0.47 |
| 11:A:920:U:H2' | 11:A:921:U:C6 | 2.49 | 0.47 |
| 11:A:1523:G:H2' | 11:A:1523:G:N3 | 2.30 | 0.47 |
| 2:F:18:VAL:HB | 2:F:19:PRO:HD3 | 1.97 | 0.47 |
| 4:K:45:THR:HG21 | 11:A:688:G:O3' | 2.15 | 0.47 |
| 9:R:62:ARG:HA | 9:R:67:LEU:O | 2.15 | 0.47 |
| 11:A:9:G:H2' | 11:A:10:A:H8 | 1.80 | 0.47 |
| 11:A:493:A:H5' | 11:A:494:G:OP2 | 2.15 | 0.47 |
| 3:H:5:PRO:O | 3:H:8:ASP:HB3 | 2.15 | 0.47 |
| 9:R:42:ARG:HH22 | 11:A:721:G:P | 2.38 | 0.47 |
| 11:A:864:A:H2' | 11:A:865:A:C8 | 2.50 | 0.47 |
| 11:A:1502:A:C5 | 11:A:1530:G:H4' | 2.50 | 0.47 |
| 2:F:4:TYR:HA | 2:F:90:MET:O | 2.15 | 0.46 |
| 3:H:12:ARG:NH1 | 11:A:826:C:H5' | 2.30 | 0.46 |
| 4:K:12:ARG:HH12 | 11:A:684:U:HO2' | 1.63 | 0.46 |
| 11:A:88:U:HO2' | 11:A:89:U:H6 | 1.59 | 0.46 |
| 11:A:475:C:H2' | 11:A:476:U:H6 | 1.80 | 0.46 |
| 11:A:582:C:N3 | 11:A:759:A:N7 | 2.63 | 0.46 |
| 11:A:676:A:H2 | 11:A:715:A:N1 | 2.12 | 0.46 |
| 11:A:923:A:C5 | 11:A:924:C:H5 | 2.32 | 0.46 |
| 3:H:42:GLU:CD | 3:H:44:PHE:HD2 | 2.18 | 0.46 |
| 5:L:51:VAL:HG22 | 5:L:65:TYR:HD1 | 1.80 | 0.46 |
| 11:A:24:U:O2' | 11:A:524:G:O2' | 2.12 | 0.46 |
| 11:A:107:G:C2 | 11:A:108:G:H1' | 2.50 | 0.46 |
| 11:A:649:A:H2' | 11:A:650:G:O4' | 2.16 | 0.46 |
| 2:F:68:GLN:HG2 | 11:A:739:C:OP1 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 6:O:35:ILE:CD1 | 6:O:59:VAL:HA | 2.45 | 0.46 |
| 11:A:15:G:N7 | 11:A:1396:A:N6 | 2.63 | 0.46 |
| 11:A:38:G:H22 | 11:A:397:A:H5' | 1.80 | 0.46 |
| 11:A:90:C:H2' | 11:A:91:U:H6 | 1.80 | 0.46 |
| 11:A:604:G:H2' | 11:A:605:U:O4' | 2.15 | 0.46 |
| 11:A:774:G:H3' | 11:A:775:G:H8 | 1.80 | 0.46 |
| 1:D:149:LYS:HB3 | 1:D:177:MET:HE1 | 1.97 | 0.46 |
| 1:D:171:GLU:CG | 1:D:182:LYS:HD2 | 2.44 | 0.46 |
| 9:R:61:ALA:HA | 9:R:64:LEU:HB3 | 1.95 | 0.46 |
| 11:A:334:C:HO2' | 11:A:335:C:H5' | 1.78 | 0.46 |
| 11:A:766:A:H2 | 11:A:1525:G:N3 | 2.13 | 0.46 |
| 11:A:784:A:H2' | 11:A:784:A:N3 | 2.30 | 0.46 |
| 11:A:893:C:H2' | 11:A:894:G:H8 | 1.79 | 0.46 |
| 11:A:98:A:H2' | 11:A:99:C:C6 | 2.51 | 0.46 |
| 11:A:465:A:N6 | 11:A:468:A:C8 | 2.83 | 0.46 |
| 11:A:658:C:H2' | 11:A:659:U:C6 | 2.50 | 0.46 |
| 11:A:1518:A:H4' | 11:A:1519:A:OP1 | 2.15 | 0.46 |
| 11:A:13:U:O2 | 11:A:915:A:N7 | 2.48 | 0.46 |
| 11:A:93:U:H2' | 11:A:95:C:C5 | 2.51 | 0.46 |
| 11:A:713:G:C4 | 11:A:714:G:N1 | 2.84 | 0.46 |
| 5:L:49:ARG:NH2 | 11:A:521:G:O6 | 2.49 | 0.46 |
| 11:A:154:U:O4 | 11:A:155:A:N6 | 2.49 | 0.46 |
| 11:A:301:G:H2' | 11:A:302:G:C8 | 2.50 | 0.46 |
| 11:A:505:G:C2 | 11:A:506:G:C5 | 3.04 | 0.46 |
| 11:A:767:A:H2' | 11:A:768:A:O4' | 2.14 | 0.46 |
| 1:D:171:GLU:CD | 1:D:182:LYS:HD2 | 2.35 | 0.46 |
| 9:R:19:GLU:OE1 | 9:R:50:TYR:OH | 2.34 | 0.46 |
| 3:H:58:LEU:HD23 | 3:H:60:LEU:HB2 | 1.98 | 0.46 |
| 11:A:313:A:H2' | 11:A:314:C:C6 | 2.50 | 0.46 |
| 11:A:904:U:C2 | 11:A:905:U:C5 | 3.04 | 0.46 |
| 8:Q:29:LYS:HA | 8:Q:36:PHE:HA | 1.97 | 0.46 |
| 11:A:206:C:H2' | 11:A:207:C:C6 | 2.50 | 0.46 |
| 11:A:601:G:H2' | 11:A:602:A:H8 | 1.80 | 0.46 |
| 11:A:801:U:C2 | 11:A:802:A:C8 | 3.04 | 0.46 |
| 2:F:18:VAL:CG1 | 2:F:22:ILE:HD11 | 2.46 | 0.45 |
| 11:A:123:U:H2' | 11:A:124:C:C6 | 2.51 | 0.45 |
| 11:A:268:U:H2' | 11:A:269:C:C6 | 2.51 | 0.45 |
| 11:A:673:A:C4 | 11:A:734:G:N2 | 2.84 | 0.45 |
| 11:A:836:G:C5 | 11:A:851:G:C6 | 3.04 | 0.45 |
| 11:A:838:G:C4 | 11:A:849:G:C2 | 3.04 | 0.45 |
| 11:A:839:C:H2' | 11:A:840:C:C6 | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 11:A:844:G:H2' | 11:A:845:A:O4' | 2.16 | 0.45 |
| 1:D:25:ARG:HD3 | 1:D:30:LYS:HD3 | 1.99 | 0.45 |
| 5:L:71:HIS:CD2 | 5:L:72:ASN:N | 2.84 | 0.45 |
| 11:A:204:G:H2' | 11:A:205:A:C8 | 2.51 | 0.45 |
| 11:A:435:A:N7 | 12:A:1632:HOH:O | 2.47 | 0.45 |
| 10:T:27:MET:CG | 10:T:57:VAL:HG12 | 2.47 | 0.45 |
| 11:A:239:U:H5' | 11:A:240:G:OP2 | 2.17 | 0.45 |
| 11:A:787:A:H2' | 11:A:788:U:C6 | 2.51 | 0.45 |
| 11:A:1390:U:H2' | 11:A:1391:U:C6 | 2.51 | 0.45 |
| 11:A:1392:G:H2' | 11:A:1393:U:C6 | 2.51 | 0.45 |
| 11:A:1393:U:H2' | 11:A:1394:A:O4' | 2.16 | 0.45 |
| 5:L:47:ALA:HB2 | 11:A:529:G:H22 | 1.81 | 0.45 |
| 11:A:212:G:C2 | 11:A:213:G:C8 | 3.04 | 0.45 |
| 6:O:41:HIS:CE1 | 6:O:44:GLU:OE1 | 2.68 | 0.45 |
| 11:A:407:U:H2' | 11:A:408:A:H8 | 1.76 | 0.45 |
| 11:A:825:A:H1' | 12:A:1604:HOH:O | 2.17 | 0.45 |
| 11:A:845:A:C8 | 11:A:846:G:H8 | 2.35 | 0.45 |
| 11:A:1510:C:N3 | 11:A:1526:G:N1 | 2.64 | 0.45 |
| 6:O:35:ILE:HD13 | 6:O:59:VAL:HG22 | 1.97 | 0.45 |
| 8:Q:18:LYS:HD3 | 8:Q:48:GLU:OE2 | 2.16 | 0.45 |
| 11:A:150:U:H2' | 11:A:151:A:H8 | 1.82 | 0.45 |
| 8:Q:66:LEU:HB2 | 8:Q:70:LYS:HG2 | 1.99 | 0.45 |
| 10:T:78:LEU:HD23 | 10:T:78:LEU:HA | 1.67 | 0.45 |
| 11:A:216:U:H2' | 11:A:217:C:C6 | 2.52 | 0.45 |
| 11:A:266:G:HO2' | 11:A:267:C:H3' | 1.82 | 0.45 |
| 1:D:75:TYR:CE1 | 1:D:200:VAL:HA | 2.52 | 0.45 |
| 5:L:82:ARG:NH1 | 5:L:95:HIS:CB | 2.80 | 0.45 |
| 11:A:266:G:O2' | 11:A:268:U:OP2 | 2.33 | 0.45 |
| 11:A:459:A:OP2 | 11:A:474:G:N1 | 2.34 | 0.45 |
| 11:A:472:U:H2' | 11:A:473:U:C6 | 2.52 | 0.45 |
| 11:A:162:A:O5' | 11:A:162:A:H8 | 1.99 | 0.45 |
| 11:A:173:U:H6 | 11:A:198:G:HO2' | 1.61 | 0.45 |
| 11:A:655:A:H2' | 11:A:656:G:O4' | 2.17 | 0.45 |
| 11:A:669:G:H2' | 11:A:670:G:C8 | 2.52 | 0.45 |
| 11:A:679:C:N3 | 11:A:712:A:N1 | 2.65 | 0.45 |
| 11:A:721:G:C6 | 11:A:733:G:C2 | 3.05 | 0.45 |
| 11:A:746:A:C6 | 11:A:747:A:C6 | 3.05 | 0.45 |
| 11:A:806:C:H2' | 11:A:807:A:C8 | 2.52 | 0.45 |
| 4:K:51:PHE:HE2 | 4:K:56:LYS:HG3 | 1.80 | 0.45 |
| 8:Q:18:LYS:HE3 | 11:A:255:G:O3' | 2.17 | 0.45 |
| 11:A:678:U:H2' | 11:A:679:C:C6 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 11:A:687:A:N3 | 11:A:688:G:H1' | 2.31 | 0.45 |
| 2:F:12:PRO:HB3 | 2:F:44:ARG:HD3 | 1.98 | 0.44 |
| 4:K:22:ILE:HG22 | 4:K:24:ALA:HB2 | 1.99 | 0.44 |
| 11:A:33:A:H2' | 11:A:34:C:C6 | 2.52 | 0.44 |
| 11:A:151:A:OP2 | 11:A:169:C:N4 | 2.49 | 0.44 |
| 11:A:383:A:C5 | 11:A:384:G:H1' | 2.52 | 0.44 |
| 11:A:486:U:H2' | 11:A:487:A:H8 | 1.81 | 0.44 |
| 11:A:518:C:H2' | 11:A:530:G:C8 | 2.52 | 0.44 |
| 11:A:773:G:O6 | 11:A:807:A:N6 | 2.50 | 0.44 |
| 6:O:82:GLU:N | 6:O:82:GLU:OE1 | 2.50 | 0.44 |
| 7:P:44:SER:OG | 7:P:47:GLU:HB2 | 2.17 | 0.44 |
| 11:A:151:A:H2' | 11:A:152:A:O4' | 2.17 | 0.44 |
| 11:A:618:C:O2 | 11:A:622:A:N6 | 2.50 | 0.44 |
| 11:A:766:A:N7 | 11:A:813:U:C2 | 2.85 | 0.44 |
| 11:A:832:G:H1 | 11:A:854:U:H3 | 1.65 | 0.44 |
| 11:A:916:U:H2' | 11:A:917:G:C8 | 2.52 | 0.44 |
| 5:L:78:VAL:O | 5:L:102:ASP:HB2 | 2.17 | 0.44 |
| 11:A:1391:U:H2' | 11:A:1392:G:C8 | 2.43 | 0.44 |
| 3:H:58:LEU:CD2 | 3:H:60:LEU:HB2 | 2.47 | 0.44 |
| 8:Q:16:MET:HG2 | 11:A:275:G:O2' | 2.17 | 0.44 |
| 9:R:24:ASP:N | 9:R:24:ASP:OD1 | 2.48 | 0.44 |
| 11:A:121:U:O2' | 11:A:121:U:O2 | 2.34 | 0.44 |
| 11:A:309:A:O2' | 11:A:607:A:N1 | 2.42 | 0.44 |
| 11:A:356:A:N3 | 11:A:368:U:O2' | 2.46 | 0.44 |
| 11:A:514:C:H3' | 11:A:532:A:N6 | 2.29 | 0.44 |
| 5:L:82:ARG:NH1 | 5:L:95:HIS:HB2 | 2.33 | 0.44 |
| 8:Q:45:VAL:HG21 | 8:Q:60:ILE:HG21 | 2.00 | 0.44 |
| 11:A:51:A:N7 | 11:A:114:U:O2' | 2.49 | 0.44 |
| 11:A:189:A:H2' | 11:A:190:A:C8 | 2.53 | 0.44 |
| 11:A:359:G:H2' | 11:A:360:G:O4' | 2.17 | 0.44 |
| 2:F:2:ARG:CD | 2:F:92:THR:CG2 | 2.96 | 0.44 |
| 4:K:26:PHE:HA | 4:K:90:PRO:HD3 | 1.99 | 0.44 |
| 11:A:416:G:H2' | 11:A:417:G:H8 | 1.83 | 0.44 |
| 11:A:465:A:O3' | 11:A:466:A:C5 | 2.71 | 0.44 |
| 1:D:1:ALA:HB2 | 11:A:547:A:P | 2.57 | 0.44 |
| 6:O:48:ASP:CG | 6:O:51:SER:OG | 2.57 | 0.44 |
| 11:A:31:G:N7 | 11:A:306:A:H1' | 2.32 | 0.44 |
| 11:A:50:A:N1 | 11:A:360:G:O2' | 2.46 | 0.44 |
| 11:A:109:A:H2' | 11:A:326:G:N2 | 2.33 | 0.44 |
| 11:A:148:G:H2' | 11:A:149:A:O4' | 2.18 | 0.44 |
| 11:A:152:A:H3' | 11:A:153:C:H6 | 1.81 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 11:A:661:G:N1 | 11:A:745:G:C6 | 2.86 | 0.44 |
| 11:A:801:U:H2' | 11:A:802:A:H8 | 1.83 | 0.44 |
| 11:A:837:U:C2 | 11:A:849:G:O6 | 2.70 | 0.44 |
| 1:D:30:LYS:HE3 | 11:A:410:G:C8 | 2.53 | 0.44 |
| 1:D:94:GLU:HA | 1:D:99:ASN:ND2 | 2.32 | 0.44 |
| 1:D:112:GLU:OE2 | 1:D:153:ARG:CD | 2.50 | 0.44 |
| 2:F:17:GLN:OE1 | 2:F:20:GLY:HA3 | 2.18 | 0.44 |
| 11:A:48:C:H6 | 11:A:365:U:O4 | 2.01 | 0.44 |
| 11:A:582:C:H41 | 11:A:758:C:H2' | 1.83 | 0.44 |
| 11:A:843:U:H2' | 11:A:844:G:C5 | 2.52 | 0.44 |
| 1:D:10:LEU:HD11 | 1:D:62:ARG:HD2 | 1.99 | 0.43 |
| 1:D:149:LYS:CG | 1:D:177:MET:HE3 | 2.48 | 0.43 |
| 2:F:11:HIS:HB3 | 2:F:54:LEU:HD23 | 1.98 | 0.43 |
| 8:Q:19:SER:HB3 | 8:Q:70:LYS:HZ1 | 1.83 | 0.43 |
| 11:A:448:A:N7 | 11:A:486:U:C2 | 2.85 | 0.43 |
| 11:A:691:G:H2' | 11:A:692:U:C6 | 2.52 | 0.43 |
| 11:A:696:A:H2' | 11:A:697:U:O4' | 2.18 | 0.43 |
| 11:A:1526:G:C2 | 11:A:1527:U:C4 | 3.06 | 0.43 |
| 4:K:16:SER:O | 4:K:16:SER:OG | 2.35 | 0.43 |
| 4:K:21:HIS:ND1 | 11:A:706:A:O2' | 2.51 | 0.43 |
| 9:R:62:ARG:NH1 | 11:A:719:C:N3 | 2.48 | 0.43 |
| 10:T:53:MET:O | 10:T:53:MET:HG2 | 2.16 | 0.43 |
| 11:A:680:C:H2' | 11:A:681:A:H8 | 1.83 | 0.43 |
| 11:A:748:G:C2 | 11:A:749:A:C5 | 3.06 | 0.43 |
| 2:F:61:LEU:HG | 2:F:63:ASN:HD21 | 1.82 | 0.43 |
| 2:F:91:ARG:HH21 | 11:A:738:C:P | 2.41 | 0.43 |
| 7:P:52:LEU:HD23 | 7:P:52:LEU:HA | 1.75 | 0.43 |
| 11:A:739:C:H2' | 11:A:740:U:C6 | 2.53 | 0.43 |
| 4:K:80:ASN:HB3 | 4:K:105:ARG:NE | 2.34 | 0.43 |
| 5:L:32:VAL:HG12 | 5:L:32:VAL:O | 2.18 | 0.43 |
| 5:L:75:GLU:OE2 | 5:L:76:HIS:ND1 | 2.51 | 0.43 |
| 6:O:23:SER:HB2 | 6:O:26:VAL:HG23 | 2.00 | 0.43 |
| 6:O:32:THR:HA | 6:O:62:ARG:HH11 | 1.82 | 0.43 |
| 11:A:769:G:H4' | 11:A:1513:A:C4' | 2.42 | 0.43 |
| 11:A:1395:C:H2' | 11:A:1396:A:C8 | 2.54 | 0.43 |
| 2:F:43:GLY:HA2 | 2:F:58:HIS:CE1 | 2.53 | 0.43 |
| 6:O:66:LEU:HD13 | 6:O:87:ARG:HG2 | 1.99 | 0.43 |
| 11:A:15:G:H2' | 11:A:16:A:O4' | 2.18 | 0.43 |
| 11:A:56:U:H2' | 11:A:57:G:C8 | 2.54 | 0.43 |
| 11:A:350:G:H2' | 11:A:351:G:C8 | 2.54 | 0.43 |
| 11:A:602:A:H2' | 11:A:603:U:C6 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 11:A:830:G:H2' | 11:A:831:A:H8 | 1.84 | 0.43 |
| 1:D:44:LYS:NZ | 1:D:46:ARG:HB2 | 2.33 | 0.43 |
| 8:Q:68:LYS:O | 11:A:254:G:OP1 | 2.36 | 0.43 |
| 11:A:613:C:H2' | 11:A:614:C:C6 | 2.54 | 0.43 |
| 11:A:845:A:C8 | 11:A:846:G:C8 | 3.06 | 0.43 |
| 2:F:18:VAL:O | 2:F:22:ILE:CG1 | 2.58 | 0.43 |
| 6:O:34:GLN:O | 6:O:38:LEU:CD1 | 2.66 | 0.43 |
| 11:A:270:A:H2' | 11:A:271:C:C6 | 2.54 | 0.43 |
| 11:A:325:A:H2' | 11:A:326:G:O4' | 2.18 | 0.43 |
| 11:A:455:G:N7 | 12:A:1652:HOH:O | 2.52 | 0.43 |
| 11:A:494:G:O2' | 11:A:496:A:H1' | 2.19 | 0.43 |
| 11:A:778:G:C6 | 11:A:779:C:C4 | 3.07 | 0.43 |
| 11:A:854:U:H2' | 11:A:855:U:C6 | 2.54 | 0.43 |
| 5:L:2:THR:HG21 | 11:A:880:C:OP2 | 2.18 | 0.43 |
| 11:A:37:U:O2' | 11:A:500:G:H4' | 2.19 | 0.43 |
| 11:A:505:G:H2' | 11:A:506:G:H8 | 1.84 | 0.43 |
| 11:A:608:A:H2' | 11:A:609:A:O4' | 2.18 | 0.43 |
| 11:A:768:A:H4' | 11:A:1523:G:H22 | 1.83 | 0.43 |
| 1:D:8:LEU:CD2 | 11:A:429:U:C5' | 2.94 | 0.43 |
| 1:D:36:ALA:HB3 | 1:D:41:GLY:HA2 | 2.01 | 0.43 |
| 5:L:66:ILE:CD1 | 5:L:98:ARG:HH11 | 2.27 | 0.43 |
| 11:A:204:G:H2' | 11:A:205:A:H8 | 1.84 | 0.43 |
| 11:A:251:G:H1' | 11:A:266:G:N7 | 2.34 | 0.43 |
| 11:A:301:G:H2' | 11:A:302:G:H8 | 1.84 | 0.43 |
| 11:A:343:U:H2' | 11:A:345:C:C5 | 2.54 | 0.43 |
| 1:D:2:ARG:O | 1:D:4:LEU:CD1 | 2.67 | 0.43 |
| 5:L:47:ALA:O | 5:L:49:ARG:HG3 | 2.19 | 0.43 |
| 6:O:81:ILE:HG13 | 6:O:82:GLU:CD | 2.39 | 0.43 |
| 10:T:2:ASN:ND2 | 10:T:7:LYS:HG2 | 2.32 | 0.43 |
| 11:A:212:G:N3 | 11:A:213:G:C8 | 2.87 | 0.43 |
| 11:A:473:U:N3 | 11:A:474:G:C8 | 2.87 | 0.43 |
| 11:A:517:G:O6 | 11:A:532:A:C8 | 2.71 | 0.43 |
| 11:A:782:A:H5' | 11:A:783:C:OP2 | 2.18 | 0.43 |
| 11:A:786:G:C6 | 11:A:787:A:N1 | 2.87 | 0.43 |
| 11:A:860:A:H2' | 11:A:861:G:O4' | 2.19 | 0.43 |
| 5:L:5:GLN:NE2 | 11:A:881:G:N7 | 2.64 | 0.42 |
| 5:L:23:LEU:HD13 | 5:L:94:TYR:CE1 | 2.54 | 0.42 |
| 7:P:70:ARG:O | 7:P:74:LEU:CG | 2.61 | 0.42 |
| 11:A:182:A:O2' | 11:A:183:C:H3' | 2.19 | 0.42 |
| 11:A:771:G:C6 | 11:A:809:G:C6 | 3.07 | 0.42 |
| 11:A:825:A:H2' | 11:A:826:C:C6 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 11:A:902:G:C4 | 11:A:903:G:C8 | 3.06 | 0.42 |
| 1:D:14:GLU:HG3 | 1:D:18:LEU:HD11 | 2.01 | 0.42 |
| 1:D:17:ASP:OD1 | 1:D:18:LEU:N | 2.52 | 0.42 |
| 11:A:255:G:H2' | 11:A:256:U:C6 | 2.54 | 0.42 |
| 11:A:284:C:H2' | 11:A:285:C:H6 | 1.84 | 0.42 |
| 11:A:411:A:N1 | 11:A:430:A:C5 | 2.86 | 0.42 |
| 11:A:1519:A:C8 | 11:A:1520:C:C5 | 3.06 | 0.42 |
| 5:L:110:LYS:HB2 | 11:A:538:G:H5'' | 2.00 | 0.42 |
| 11:A:201:G:H2' | 11:A:202:G:O4' | 2.18 | 0.42 |
| 11:A:253:A:H2' | 11:A:254:G:C8 | 2.54 | 0.42 |
| 11:A:398:U:H2' | 11:A:399:G:C8 | 2.54 | 0.42 |
| 11:A:459:A:H61 | 11:A:472:U:H3 | 1.65 | 0.42 |
| 11:A:833:G:C6 | 11:A:834:U:C4 | 3.07 | 0.42 |
| 11:A:894:G:C4 | 11:A:895:G:C8 | 3.07 | 0.42 |
| 11:A:1519:A:O2' | 11:A:1520:C:H6 | 2.02 | 0.42 |
| 5:L:56:LEU:HD11 | 5:L:81:ILE:HD11 | 2.01 | 0.42 |
| 11:A:76:G:O6 | 11:A:93:U:C4 | 2.72 | 0.42 |
| 11:A:130:A:H1' | 11:A:263:A:O2' | 2.20 | 0.42 |
| 11:A:461:A:O2' | 11:A:467:U:OP1 | 2.32 | 0.42 |
| 11:A:829:G:O6 | 11:A:857:C:N4 | 2.31 | 0.42 |
| 11:A:896:C:H2' | 11:A:897:C:C6 | 2.54 | 0.42 |
| 1:D:139:ASN:N | 1:D:181:PHE:O | 2.42 | 0.42 |
| 10:T:14:GLU:HG3 | 12:T:103:HOH:O | 2.19 | 0.42 |
| 11:A:89:U:H2' | 11:A:90:C:H6 | 1.81 | 0.42 |
| 11:A:441:A:H61 | 11:A:493:A:H61 | 1.62 | 0.42 |
| 11:A:455:G:H8 | 12:A:1652:HOH:O | 1.97 | 0.42 |
| 11:A:560:A:H4' | 11:A:561:U:H5'' | 2.01 | 0.42 |
| 11:A:688:G:C2 | 11:A:689:C:C5 | 3.08 | 0.42 |
| 1:D:53:GLN:O | 1:D:56:GLU:HG3 | 2.20 | 0.42 |
| 4:K:13:LYS:NZ | 4:K:35:ASP:OD2 | 2.38 | 0.42 |
| 6:O:14:PHE:CE2 | 6:O:84:LEU:HD13 | 2.54 | 0.42 |
| 8:Q:46:HIS:HB2 | 8:Q:70:LYS:HE3 | 2.02 | 0.42 |
| 11:A:28:A:H2' | 11:A:29:U:O4' | 2.20 | 0.42 |
| 11:A:155:A:N6 | 11:A:167:A:N6 | 2.68 | 0.42 |
| 11:A:680:C:H2' | 11:A:681:A:C8 | 2.54 | 0.42 |
| 11:A:816:A:OP2 | 11:A:817:C:H2' | 2.19 | 0.42 |
| 11:A:832:G:C2 | 11:A:833:G:C4 | 3.07 | 0.42 |
| 1:D:195:ASN:OD1 | 1:D:197:HIS:CE1 | 2.72 | 0.42 |
| 3:H:91:LEU:HD23 | 3:H:91:LEU:HA | 1.89 | 0.42 |
| 7:P:6:LEU:HD22 | 7:P:17:TYR:HB3 | 2.01 | 0.42 |
| 8:Q:8:GLN:HE21 | 8:Q:78:VAL:HG21 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 10:T:55:PRO:HG3 | 11:A:193:C:H4' | 2.01 | 0.42 |
| 11:A:202:G:H21 | 11:A:465:A:N6 | 2.18 | 0.42 |
| 11:A:205:A:C5 | 11:A:206:C:C5 | 3.08 | 0.42 |
| 11:A:264:C:H2' | 11:A:265:G:O4' | 2.20 | 0.42 |
| 11:A:398:U:H2' | 11:A:399:G:H8 | 1.84 | 0.42 |
| 11:A:688:G:N2 | 11:A:700:G:H1' | 2.34 | 0.42 |
| 1:D:33:ILE:CG2 | 1:D:34:GLU:N | 2.69 | 0.42 |
| 1:D:160:LEU:HD12 | 1:D:160:LEU:O | 2.20 | 0.42 |
| 11:A:160:A:H8 | 11:A:160:A:OP1 | 2.02 | 0.42 |
| 11:A:197:A:N1 | 11:A:220:G:O2' | 2.46 | 0.42 |
| 11:A:459:A:H2' | 11:A:460:A:C8 | 2.52 | 0.42 |
| 11:A:516:U:O4 | 11:A:532:A:C8 | 2.72 | 0.42 |
| 11:A:767:A:H2' | 11:A:768:A:H8 | 1.85 | 0.42 |
| 11:A:1526:G:H2' | 11:A:1527:U:H6 | 1.82 | 0.42 |
| 1:D:149:LYS:HG2 | 1:D:177:MET:HE3 | 2.02 | 0.42 |
| 6:O:32:THR:CG2 | 6:O:84:LEU:HD21 | 2.49 | 0.42 |
| 11:A:15:G:C4 | 11:A:16:A:C8 | 3.08 | 0.42 |
| 11:A:89:U:C2 | 11:A:90:C:C5 | 3.08 | 0.42 |
| 11:A:203:G:O2' | 11:A:204:G:H8 | 2.02 | 0.42 |
| 11:A:409:U:H2' | 11:A:410:G:C8 | 2.54 | 0.42 |
| 11:A:667:G:OP1 | 11:A:732:C:O2' | 2.25 | 0.42 |
| 11:A:714:G:H2' | 11:A:715:A:C8 | 2.54 | 0.42 |
| 11:A:810:C:H1' | 11:A:899:C:H41 | 1.85 | 0.42 |
| 10:T:2:ASN:ND2 | 10:T:7:LYS:HE2 | 2.35 | 0.42 |
| 11:A:27:G:H2' | 11:A:28:A:C8 | 2.53 | 0.42 |
| 11:A:88:U:O2' | 11:A:89:U:H6 | 2.02 | 0.42 |
| 11:A:1507:A:O2' | 11:A:1508:A:OP1 | 2.33 | 0.42 |
| 11:A:71:A:N1 | 11:A:99:C:O2' | 2.49 | 0.41 |
| 11:A:749:A:H2' | 11:A:750:C:O4' | 2.19 | 0.41 |
| 11:A:779:C:OP2 | 11:A:780:A:N6 | 2.53 | 0.41 |
| 11:A:843:U:H2' | 11:A:844:G:C4 | 2.55 | 0.41 |
| 2:F:37:HIS:CD2 | 2:F:38:ARG:HE | 2.38 | 0.41 |
| 3:H:29:SER:HB3 | 11:A:589:U:H5'' | 2.02 | 0.41 |
| 5:L:33:CYS:N | 5:L:54:VAL:HG23 | 2.32 | 0.41 |
| 8:Q:5:ARG:NH2 | 11:A:636:U:H5' | 2.35 | 0.41 |
| 9:R:25:ILE:HG13 | 9:R:29:LYS:HE2 | 2.01 | 0.41 |
| 1:D:7:LYS:HB3 | 1:D:20:LEU:HD12 | 2.03 | 0.41 |
| 2:F:36:ILE:HD13 | 2:F:62:MET:HE2 | 2.00 | 0.41 |
| 2:F:57:ALA:HB3 | 2:F:59:TYR:CE1 | 2.55 | 0.41 |
| 6:O:22:GLY:O | 11:A:751:U:H1' | 2.21 | 0.41 |
| 6:O:75:ALA:HA | 6:O:78:THR:HG22 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 11:A:335:C:O2' | 11:A:336:A:P | 2.78 | 0.41 |
| 11:A:712:A:C2 | 11:A:713:G:N2 | 2.89 | 0.41 |
| 2:F:49:TYR:OH | 9:R:62:ARG:O | 2.30 | 0.41 |
| 11:A:123:U:H2' | 11:A:124:C:H6 | 1.85 | 0.41 |
| 11:A:155:A:C6 | 11:A:167:A:C6 | 3.09 | 0.41 |
| 11:A:517:G:C6 | 11:A:532:A:H8 | 2.38 | 0.41 |
| 11:A:573:A:O2' | 11:A:574:A:H5' | 2.20 | 0.41 |
| 11:A:669:G:N1 | 11:A:738:C:C4 | 2.88 | 0.41 |
| 11:A:832:G:C2 | 11:A:855:U:C2 | 3.09 | 0.41 |
| 3:H:102:VAL:HG13 | 3:H:125:ILE:HB | 2.02 | 0.41 |
| 11:A:121:U:O2' | 11:A:122:G:OP1 | 2.29 | 0.41 |
| 11:A:169:C:H2' | 11:A:170:U:C6 | 2.55 | 0.41 |
| 11:A:263:A:H2' | 11:A:264:C:C6 | 2.56 | 0.41 |
| 11:A:323:U:H2' | 11:A:324:G:O4' | 2.19 | 0.41 |
| 11:A:600:A:H2' | 11:A:601:G:C8 | 2.55 | 0.41 |
| 11:A:785:G:C2 | 11:A:786:G:C5 | 3.08 | 0.41 |
| 11:A:1523:G:C4 | 11:A:1524:C:C5 | 3.08 | 0.41 |
| 2:F:75:GLU:HA | 2:F:78:PHE:CD2 | 2.55 | 0.41 |
| 3:H:82:LEU:HD11 | 8:Q:33:TYR:O | 2.19 | 0.41 |
| 11:A:13:U:C2 | 11:A:915:A:N7 | 2.89 | 0.41 |
| 11:A:683:G:H2' | 11:A:684:U:C6 | 2.55 | 0.41 |
| 11:A:832:G:H2' | 11:A:833:G:H8 | 1.84 | 0.41 |
| 11:A:1507:A:O2' | 11:A:1508:A:P | 2.79 | 0.41 |
| 1:D:118:SER:HB2 | 12:A:1727:HOH:O | 2.19 | 0.41 |
| 5:L:97:VAL:HG12 | 5:L:100:ALA:CB | 2.48 | 0.41 |
| 11:A:22:G:H2' | 11:A:23:C:H6 | 1.86 | 0.41 |
| 11:A:96:U:H2' | 11:A:97:G:H8 | 1.86 | 0.41 |
| 11:A:444:G:C6 | 11:A:490:C:N3 | 2.86 | 0.41 |
| 11:A:466:A:O5' | 11:A:467:U:H5 | 2.02 | 0.41 |
| 11:A:771:G:C6 | 11:A:772:U:C4 | 3.08 | 0.41 |
| 11:A:838:G:C6 | 11:A:849:G:C5 | 3.09 | 0.41 |
| 1:D:103:ARG:C | 1:D:105:GLY:H | 2.24 | 0.41 |
| 2:F:26:THR:HG22 | 2:F:62:MET:HE1 | 2.03 | 0.41 |
| 2:F:68:GLN:HG2 | 11:A:739:C:P | 2.61 | 0.41 |
| 5:L:98:ARG:NH2 | 5:L:106:VAL:HG12 | 2.33 | 0.41 |
| 11:A:390:U:H2' | 11:A:391:G:C8 | 2.56 | 0.41 |
| 11:A:487:A:H2' | 11:A:488:C:O4' | 2.20 | 0.41 |
| 11:A:661:G:H2' | 11:A:662:U:C6 | 2.56 | 0.41 |
| 11:A:665:A:H1' | 11:A:733:G:O4' | 2.21 | 0.41 |
| 11:A:707:U:H2' | 11:A:708:C:C6 | 2.56 | 0.41 |
| 11:A:722:G:H3' | 11:A:722:G:N3 | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 11:A:780:A:H2 | 11:A:803:G:O6 | 2.03 | 0.41 |
| 11:A:806:C:H2' | 11:A:807:A:H8 | 1.86 | 0.41 |
| 1:D:13:ARG:HD3 | 11:A:543:U:OP1 | 2.21 | 0.41 |
| 3:H:34:ALA:HB1 | 3:H:109:VAL:HB | 2.02 | 0.41 |
| 3:H:115:ALA:HB1 | 3:H:120:LEU:O | 2.21 | 0.41 |
| 4:K:79:LYS:O | 4:K:104:PHE:HA | 2.21 | 0.41 |
| 9:R:50:TYR:HA | 9:R:53:GLN:OE1 | 2.21 | 0.41 |
| 10:T:60:GLN:OE1 | 10:T:60:GLN:HA | 2.20 | 0.41 |
| 11:A:62:U:OP1 | 11:A:385:C:O2' | 2.30 | 0.41 |
| 11:A:426:U:H2' | 11:A:427:U:C6 | 2.56 | 0.41 |
| 11:A:573:A:N3 | 11:A:883:C:O2' | 2.52 | 0.41 |
| 11:A:846:G:H3' | 11:A:847:G:H8 | 1.85 | 0.41 |
| 3:H:80:PRO:O | 11:A:878:A:H5'' | 2.21 | 0.41 |
| 11:A:75:G:C6 | 11:A:76:G:C5 | 3.08 | 0.41 |
| 11:A:334:C:C2' | 11:A:335:C:H5' | 2.51 | 0.41 |
| 1:D:4:LEU:CD2 | 11:A:406:G:H5' | 2.50 | 0.40 |
| 1:D:120:LYS:HG3 | 11:A:439:U:H5' | 2.02 | 0.40 |
| 4:K:41:LEU:HB3 | 4:K:76:TYR:CD2 | 2.56 | 0.40 |
| 5:L:55:ARG:HG2 | 5:L:55:ARG:NH1 | 2.36 | 0.40 |
| 5:L:71:HIS:HD2 | 5:L:72:ASN:N | 2.18 | 0.40 |
| 11:A:295:C:H2' | 11:A:296:U:O4' | 2.21 | 0.40 |
| 11:A:399:G:H2' | 11:A:400:C:C6 | 2.56 | 0.40 |
| 11:A:473:U:H2' | 11:A:474:G:H5' | 2.03 | 0.40 |
| 1:D:17:ASP:CG | 1:D:27:ILE:HD11 | 2.41 | 0.40 |
| 3:H:4:ASP:OD1 | 3:H:80:PRO:HD3 | 2.21 | 0.40 |
| 5:L:107:LYS:HD3 | 5:L:107:LYS:N | 2.35 | 0.40 |
| 6:O:4:THR:HG23 | 11:A:659:U:H5'' | 2.03 | 0.40 |
| 7:P:14:ARG:CB | 7:P:42:ILE:HD11 | 2.51 | 0.40 |
| 11:A:79:G:C6 | 11:A:80:A:C6 | 3.09 | 0.40 |
| 11:A:180:U:C2' | 11:A:181:A:H5' | 2.50 | 0.40 |
| 11:A:679:C:H2' | 11:A:680:C:C6 | 2.56 | 0.40 |
| 11:A:685:G:N1 | 11:A:704:A:OP2 | 2.45 | 0.40 |
| 1:D:8:LEU:HD23 | 1:D:31:CYS:HB2 | 2.02 | 0.40 |
| 1:D:10:LEU:CG | 1:D:62:ARG:HD2 | 2.51 | 0.40 |
| 4:K:40:ALA:O | 11:A:684:U:O2' | 2.23 | 0.40 |
| 4:K:49:SER:HB2 | 4:K:68:ARG:NH1 | 2.36 | 0.40 |
| 8:Q:57:VAL:HG12 | 8:Q:78:VAL:CG2 | 2.52 | 0.40 |
| 9:R:51:GLN:HE22 | 9:R:54:LEU:HD23 | 1.85 | 0.40 |
| 11:A:76:G:N2 | 11:A:93:U:O2 | 2.41 | 0.40 |
| 11:A:204:G:C6 | 11:A:205:A:C5 | 3.10 | 0.40 |
| 11:A:211:G:N1 | 11:A:212:G:C4 | 2.89 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 11:A:640:A:O2' | 11:A:641:U:H5' | 2.22 | 0.40 |
| 11:A:673:A:H2' | 11:A:674:G:H8 | 1.82 | 0.40 |
| 11:A:782:A:OP1 | 11:A:1522:U:H1' | 2.21 | 0.40 |
| 1:D:169:TRP:CD2 | 1:D:185:PRO:HB3 | 2.56 | 0.40 |
| 3:H:2:MET:HE1 | 11:A:756:C:C1' | 2.51 | 0.40 |
| 5:L:8:ARG:HH22 | 11:A:881:G:P | 2.45 | 0.40 |
| 6:O:28:VAL:HG21 | 6:O:66:LEU:HD21 | 2.03 | 0.40 |
| 11:A:70:U:H5'' | 12:A:1698:HOH:O | 2.21 | 0.40 |
| 11:A:83:C:H4' | 11:A:84:U:C5 | 2.56 | 0.40 |
| 11:A:279:A:H5' | 11:A:281:G:O4' | 2.21 | 0.40 |
| 11:A:558:G:OP2 | 11:A:559:A:O2' | 2.18 | 0.40 |
| 11:A:615:G:N2 | 12:A:1643:HOH:O | 2.49 | 0.40 |
| 11:A:697:U:O3' | 11:A:785:G:O2' | 2.36 | 0.40 |
| 11:A:706:A:C6 | 11:A:707:U:C4 | 3.09 | 0.40 |
| 11:A:903:G:C4 | 11:A:904:U:C5 | 3.10 | 0.40 |
| 1:D:120:LYS:HE3 | 1:D:130:ASN:ND2 | 2.36 | 0.40 |
| 2:F:3:HIS:CD2 | 2:F:65:GLU:HG2 | 2.57 | 0.40 |
| 6:O:68:TYR:OH | 11:A:752:G:H5'' | 2.22 | 0.40 |
| 9:R:24:ASP:O | 9:R:28:LEU:HG | 2.21 | 0.40 |
| 11:A:17:U:O2' | 11:A:18:C:OP1 | 2.36 | 0.40 |
| 11:A:80:A:H2' | 11:A:81:A:O4' | 2.22 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1 | D | 203/205 (99%) | 177 (87%) | 26 (13%) | 0 | 100 | 100 |
| 2 | F | 98/135 (73%) | 92 (94%) | 6 (6%) | 0 | 100 | 100 |
| 3 | H | 127/129 (98%) | 117 (92%) | 10 (8%) | 0 | 100 | 100 |
| 4 | K | 93/128 (73%) | 83 (89%) | 10 (11%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|-----------|-----------|----------|-------------|-----|
| 5 | L | 121/123 (98%) | 102 (84%) | 19 (16%) | 0 | 100 | 100 |
| 6 | O | 86/89 (97%) | 82 (95%) | 4 (5%) | 0 | 100 | 100 |
| 7 | P | 80/82 (98%) | 70 (88%) | 10 (12%) | 0 | 100 | 100 |
| 8 | Q | 78/83 (94%) | 68 (87%) | 10 (13%) | 0 | 100 | 100 |
| 9 | R | 48/74 (65%) | 41 (85%) | 7 (15%) | 0 | 100 | 100 |
| 10 | T | 83/86 (96%) | 81 (98%) | 2 (2%) | 0 | 100 | 100 |
| All | All | 1017/1134 (90%) | 913 (90%) | 104 (10%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 1 | D | 172/172 (100%) | 169 (98%) | 3 (2%) | 60 | 76 |
| 2 | F | 87/116 (75%) | 86 (99%) | 1 (1%) | 73 | 84 |
| 3 | H | 104/104 (100%) | 102 (98%) | 2 (2%) | 57 | 73 |
| 4 | K | 69/98 (70%) | 68 (99%) | 1 (1%) | 67 | 79 |
| 5 | L | 103/103 (100%) | 102 (99%) | 1 (1%) | 76 | 85 |
| 6 | O | 76/77 (99%) | 76 (100%) | 0 | 100 | 100 |
| 7 | P | 65/65 (100%) | 65 (100%) | 0 | 100 | 100 |
| 8 | Q | 74/77 (96%) | 74 (100%) | 0 | 100 | 100 |
| 9 | R | 43/64 (67%) | 43 (100%) | 0 | 100 | 100 |
| 10 | T | 65/65 (100%) | 65 (100%) | 0 | 100 | 100 |
| All | All | 858/941 (91%) | 850 (99%) | 8 (1%) | 79 | 87 |

All (8) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 8 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 44 | LYS |
| 1 | D | 150 | LYS |
| 2 | F | 35 | LYS |
| 3 | H | 88 | LYS |
| 3 | H | 113 | ARG |
| 4 | K | 55 | ARG |
| 5 | L | 95 | HIS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 99 | ASN |
| 1 | D | 197 | HIS |
| 2 | F | 63 | ASN |
| 4 | K | 100 | ASN |
| 5 | L | 71 | HIS |
| 6 | O | 41 | HIS |
| 6 | O | 45 | HIS |
| 8 | Q | 8 | GLN |
| 10 | T | 69 | ASN |

5.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|----------------|-------------------|-----------------|
| 11 | A | 960/1542 (62%) | 259 (26%) | 24 (2%) |

All (259) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | A | 9 | G |
| 11 | A | 14 | U |
| 11 | A | 18 | C |
| 11 | A | 20 | U |
| 11 | A | 25 | C |
| 11 | A | 32 | A |
| 11 | A | 33 | A |
| 11 | A | 35 | G |
| 11 | A | 39 | G |
| 11 | A | 44 | A |
| 11 | A | 47 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 11 | A | 48 | C |
| 11 | A | 49 | U |
| 11 | A | 50 | A |
| 11 | A | 51 | A |
| 11 | A | 54 | C |
| 11 | A | 64 | G |
| 11 | A | 65 | A |
| 11 | A | 66 | A |
| 11 | A | 70 | U |
| 11 | A | 71 | A |
| 11 | A | 72 | A |
| 11 | A | 76 | G |
| 11 | A | 77 | A |
| 11 | A | 79 | G |
| 11 | A | 80 | A |
| 11 | A | 84 | U |
| 11 | A | 85 | U |
| 11 | A | 86 | G |
| 11 | A | 87 | C |
| 11 | A | 89 | U |
| 11 | A | 90 | C |
| 11 | A | 91 | U |
| 11 | A | 93 | U |
| 11 | A | 94 | G |
| 11 | A | 95 | C |
| 11 | A | 98 | A |
| 11 | A | 100 | G |
| 11 | A | 109 | A |
| 11 | A | 110 | C |
| 11 | A | 115 | G |
| 11 | A | 116 | A |
| 11 | A | 121 | U |
| 11 | A | 122 | G |
| 11 | A | 129 | A |
| 11 | A | 130 | A |
| 11 | A | 131 | A |
| 11 | A | 133 | U |
| 11 | A | 134 | G |
| 11 | A | 144 | G |
| 11 | A | 149 | A |
| 11 | A | 151 | A |
| 11 | A | 158 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 11 | A | 159 | G |
| 11 | A | 164 | G |
| 11 | A | 173 | U |
| 11 | A | 177 | G |
| 11 | A | 181 | A |
| 11 | A | 182 | A |
| 11 | A | 183 | C |
| 11 | A | 184 | G |
| 11 | A | 195 | A |
| 11 | A | 196 | A |
| 11 | A | 197 | A |
| 11 | A | 205 | A |
| 11 | A | 209 | U |
| 11 | A | 211 | G |
| 11 | A | 222 | C |
| 11 | A | 225 | C |
| 11 | A | 239 | U |
| 11 | A | 240 | G |
| 11 | A | 243 | A |
| 11 | A | 244 | U |
| 11 | A | 245 | U |
| 11 | A | 247 | G |
| 11 | A | 251 | G |
| 11 | A | 258 | G |
| 11 | A | 266 | G |
| 11 | A | 267 | C |
| 11 | A | 279 | A |
| 11 | A | 280 | C |
| 11 | A | 289 | G |
| 11 | A | 296 | U |
| 11 | A | 298 | A |
| 11 | A | 301 | G |
| 11 | A | 305 | G |
| 11 | A | 306 | A |
| 11 | A | 321 | A |
| 11 | A | 323 | U |
| 11 | A | 328 | C |
| 11 | A | 329 | A |
| 11 | A | 332 | G |
| 11 | A | 335 | C |
| 11 | A | 336 | A |
| 11 | A | 338 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 11 | A | 345 | C |
| 11 | A | 346 | G |
| 11 | A | 352 | C |
| 11 | A | 353 | A |
| 11 | A | 354 | G |
| 11 | A | 363 | A |
| 11 | A | 364 | A |
| 11 | A | 367 | U |
| 11 | A | 369 | G |
| 11 | A | 372 | C |
| 11 | A | 378 | G |
| 11 | A | 384 | G |
| 11 | A | 397 | A |
| 11 | A | 398 | U |
| 11 | A | 406 | G |
| 11 | A | 410 | G |
| 11 | A | 411 | A |
| 11 | A | 412 | A |
| 11 | A | 413 | G |
| 11 | A | 414 | A |
| 11 | A | 415 | A |
| 11 | A | 421 | U |
| 11 | A | 422 | C |
| 11 | A | 423 | G |
| 11 | A | 424 | G |
| 11 | A | 429 | U |
| 11 | A | 430 | A |
| 11 | A | 435 | A |
| 11 | A | 438 | U |
| 11 | A | 439 | U |
| 11 | A | 446 | G |
| 11 | A | 450 | G |
| 11 | A | 451 | A |
| 11 | A | 453 | G |
| 11 | A | 457 | G |
| 11 | A | 458 | U |
| 11 | A | 459 | A |
| 11 | A | 461 | A |
| 11 | A | 462 | G |
| 11 | A | 463 | U |
| 11 | A | 464 | U |
| 11 | A | 465 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 11 | A | 466 | A |
| 11 | A | 467 | U |
| 11 | A | 468 | A |
| 11 | A | 473 | U |
| 11 | A | 475 | C |
| 11 | A | 482 | A |
| 11 | A | 484 | G |
| 11 | A | 486 | U |
| 11 | A | 488 | C |
| 11 | A | 492 | C |
| 11 | A | 493 | A |
| 11 | A | 495 | A |
| 11 | A | 508 | U |
| 11 | A | 509 | A |
| 11 | A | 511 | C |
| 11 | A | 517 | G |
| 11 | A | 518 | C |
| 11 | A | 521 | G |
| 11 | A | 522 | C |
| 11 | A | 527 | G |
| 11 | A | 532 | A |
| 11 | A | 533 | A |
| 11 | A | 536 | C |
| 11 | A | 537 | G |
| 11 | A | 547 | A |
| 11 | A | 560 | A |
| 11 | A | 564 | C |
| 11 | A | 572 | A |
| 11 | A | 573 | A |
| 11 | A | 576 | C |
| 11 | A | 577 | G |
| 11 | A | 588 | G |
| 11 | A | 596 | A |
| 11 | A | 607 | A |
| 11 | A | 615 | G |
| 11 | A | 618 | C |
| 11 | A | 619 | U |
| 11 | A | 620 | C |
| 11 | A | 642 | A |
| 11 | A | 650 | G |
| 11 | A | 653 | U |
| 11 | A | 656 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 11 | A | 660 | C |
| 11 | A | 662 | U |
| 11 | A | 665 | A |
| 11 | A | 671 | G |
| 11 | A | 673 | A |
| 11 | A | 682 | G |
| 11 | A | 685 | G |
| 11 | A | 687 | A |
| 11 | A | 689 | C |
| 11 | A | 695 | A |
| 11 | A | 698 | G |
| 11 | A | 701 | U |
| 11 | A | 702 | A |
| 11 | A | 703 | G |
| 11 | A | 710 | G |
| 11 | A | 713 | G |
| 11 | A | 714 | G |
| 11 | A | 719 | C |
| 11 | A | 721 | G |
| 11 | A | 723 | U |
| 11 | A | 724 | G |
| 11 | A | 729 | A |
| 11 | A | 731 | G |
| 11 | A | 734 | G |
| 11 | A | 747 | A |
| 11 | A | 748 | G |
| 11 | A | 755 | G |
| 11 | A | 759 | A |
| 11 | A | 770 | C |
| 11 | A | 771 | G |
| 11 | A | 776 | G |
| 11 | A | 777 | A |
| 11 | A | 782 | A |
| 11 | A | 785 | G |
| 11 | A | 790 | A |
| 11 | A | 791 | G |
| 11 | A | 793 | U |
| 11 | A | 794 | A |
| 11 | A | 811 | C |
| 11 | A | 812 | G |
| 11 | A | 813 | U |
| 11 | A | 814 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 11 | A | 815 | A |
| 11 | A | 816 | A |
| 11 | A | 817 | C |
| 11 | A | 818 | G |
| 11 | A | 820 | U |
| 11 | A | 821 | G |
| 11 | A | 828 | U |
| 11 | A | 829 | G |
| 11 | A | 835 | U |
| 11 | A | 836 | G |
| 11 | A | 841 | C |
| 11 | A | 842 | U |
| 11 | A | 843 | U |
| 11 | A | 844 | G |
| 11 | A | 846 | G |
| 11 | A | 847 | G |
| 11 | A | 871 | U |
| 11 | A | 874 | G |
| 11 | A | 876 | C |
| 11 | A | 900 | A |
| 11 | A | 902 | G |
| 11 | A | 904 | U |
| 11 | A | 914 | A |
| 11 | A | 923 | A |
| 11 | A | 928 | G |
| 11 | A | 1390 | U |
| 11 | A | 1502 | A |
| 11 | A | 1503 | A |
| 11 | A | 1504 | G |
| 11 | A | 1505 | G |
| 11 | A | 1507 | A |
| 11 | A | 1508 | A |
| 11 | A | 1509 | C |
| 11 | A | 1519 | A |
| 11 | A | 1520 | C |
| 11 | A | 1523 | G |
| 11 | A | 1529 | G |
| 11 | A | 1530 | G |

All (24) RNA pucker outliers are listed below:

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
|-----|-------|-----|------|

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 11 | A | 17 | U |
| 11 | A | 71 | A |
| 11 | A | 86 | G |
| 11 | A | 183 | C |
| 11 | A | 243 | A |
| 11 | A | 244 | U |
| 11 | A | 266 | G |
| 11 | A | 328 | C |
| 11 | A | 410 | G |
| 11 | A | 411 | A |
| 11 | A | 412 | A |
| 11 | A | 413 | G |
| 11 | A | 414 | A |
| 11 | A | 428 | G |
| 11 | A | 429 | U |
| 11 | A | 465 | A |
| 11 | A | 532 | A |
| 11 | A | 776 | G |
| 11 | A | 812 | G |
| 11 | A | 842 | U |
| 11 | A | 843 | U |
| 11 | A | 1507 | A |
| 11 | A | 1518 | A |
| 11 | A | 1528 | U |

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

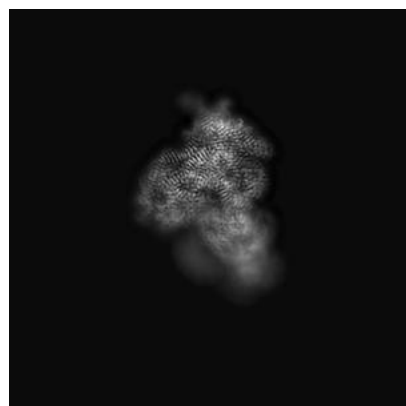
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12916. These allow visual inspection of the internal detail of the map and identification of artifacts.

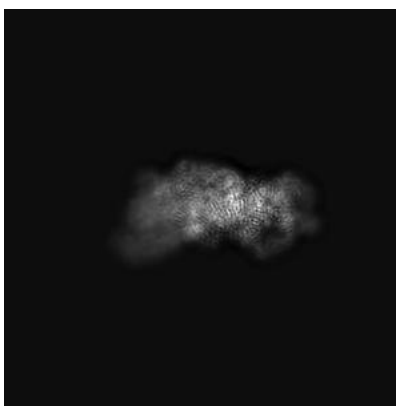
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

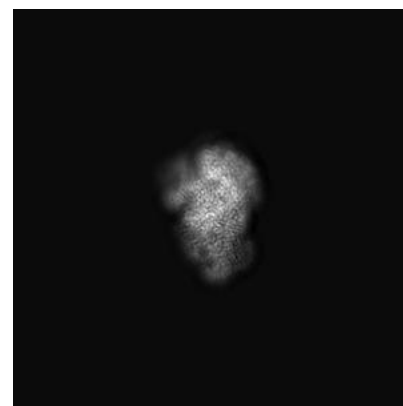
6.1.1 Primary map



X

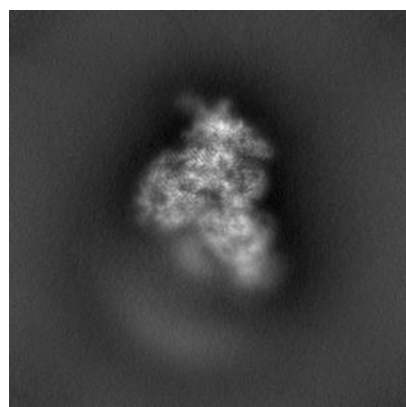


Y

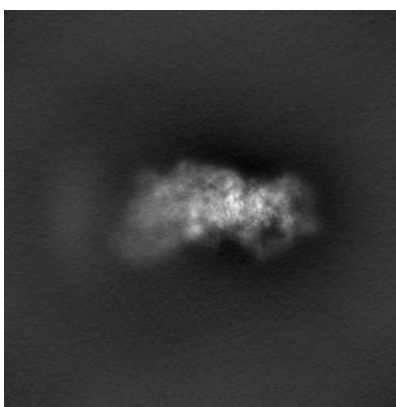


Z

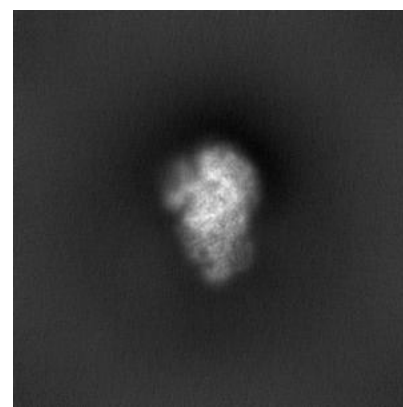
6.1.2 Raw map



X



Y

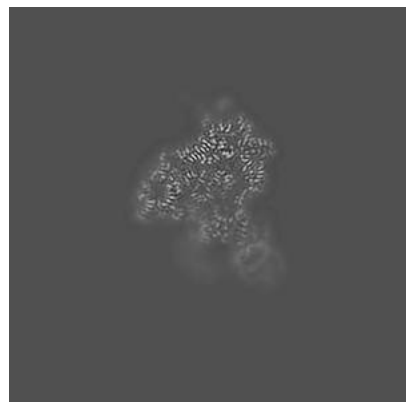


Z

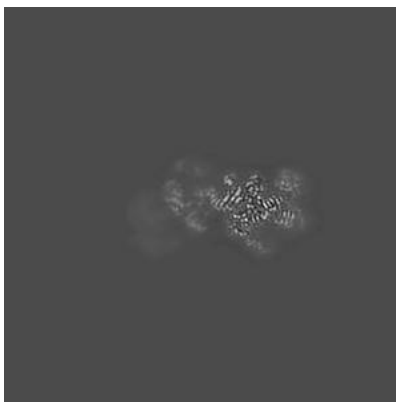
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

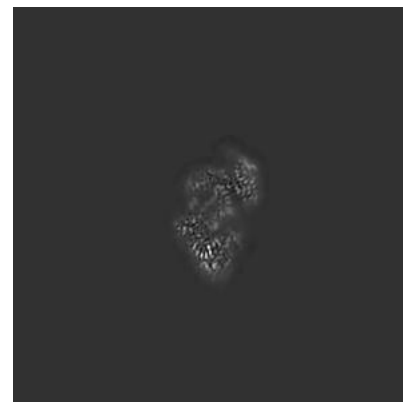
6.2.1 Primary map



X Index: 220

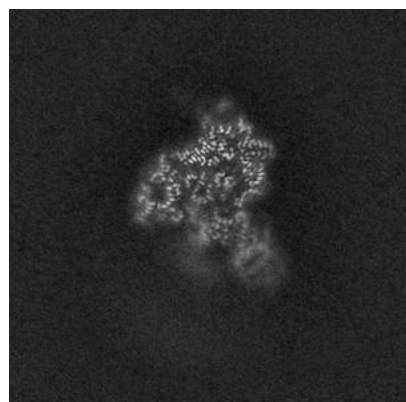


Y Index: 220

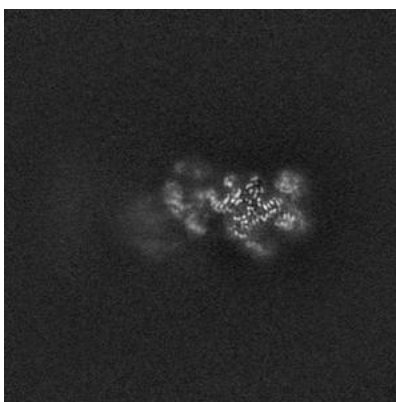


Z Index: 220

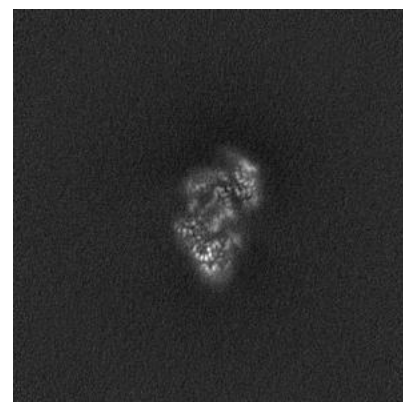
6.2.2 Raw map



X Index: 220



Y Index: 220

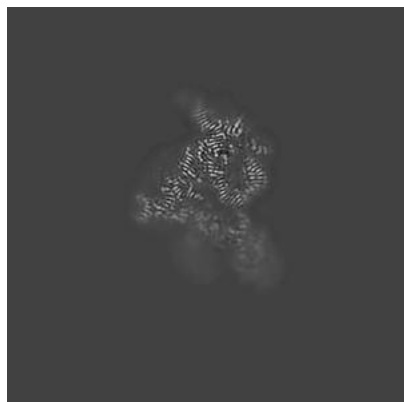


Z Index: 220

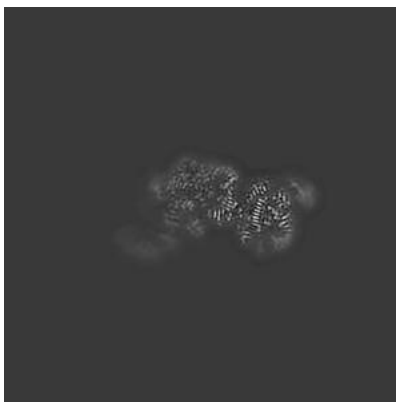
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

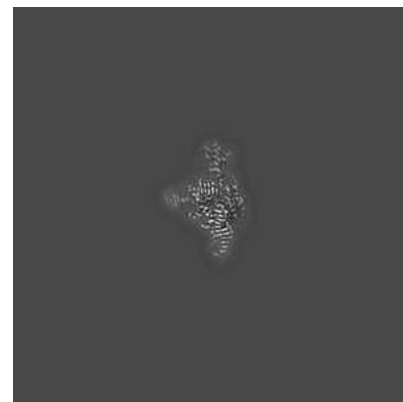
6.3.1 Primary map



X Index: 213

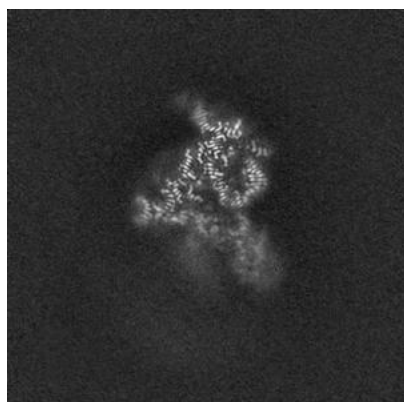


Y Index: 238

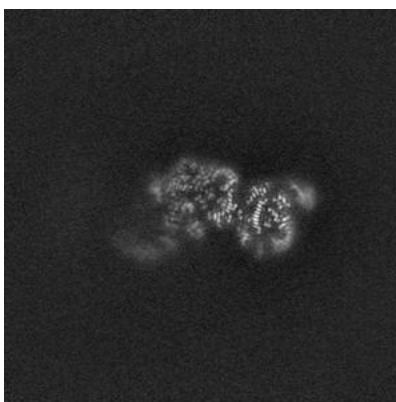


Z Index: 279

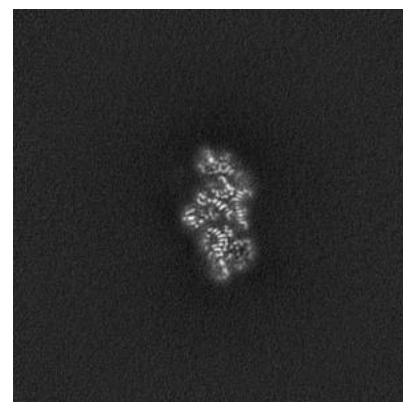
6.3.2 Raw map



X Index: 213



Y Index: 238

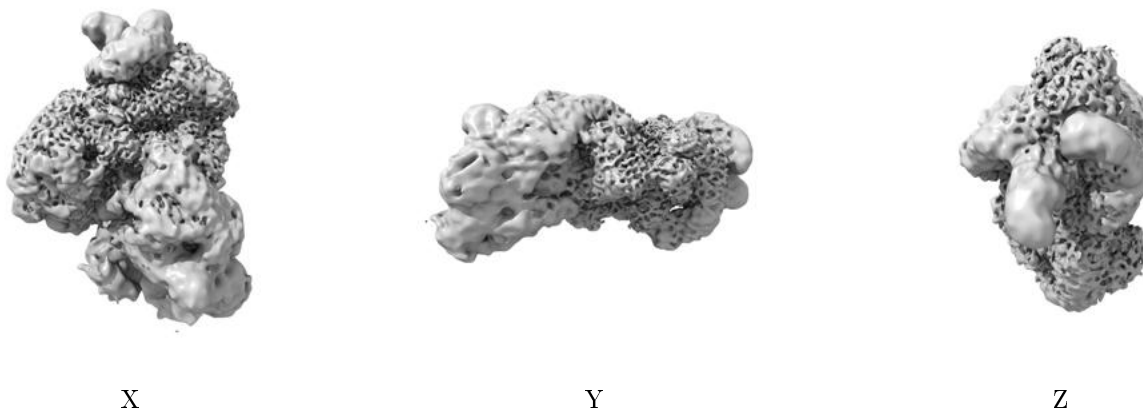


Z Index: 250

The images above show the largest variance slices of the map in three orthogonal directions.

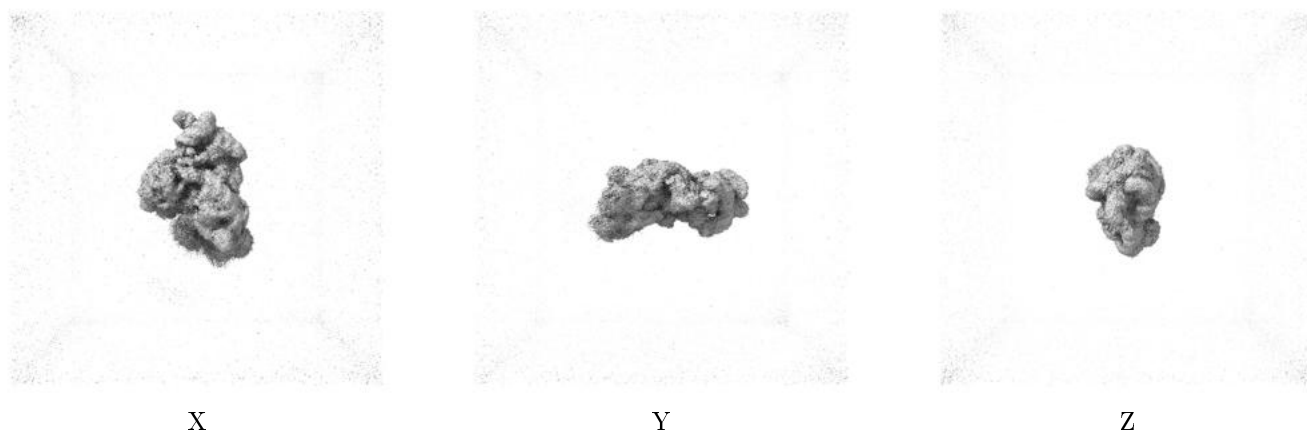
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.218. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

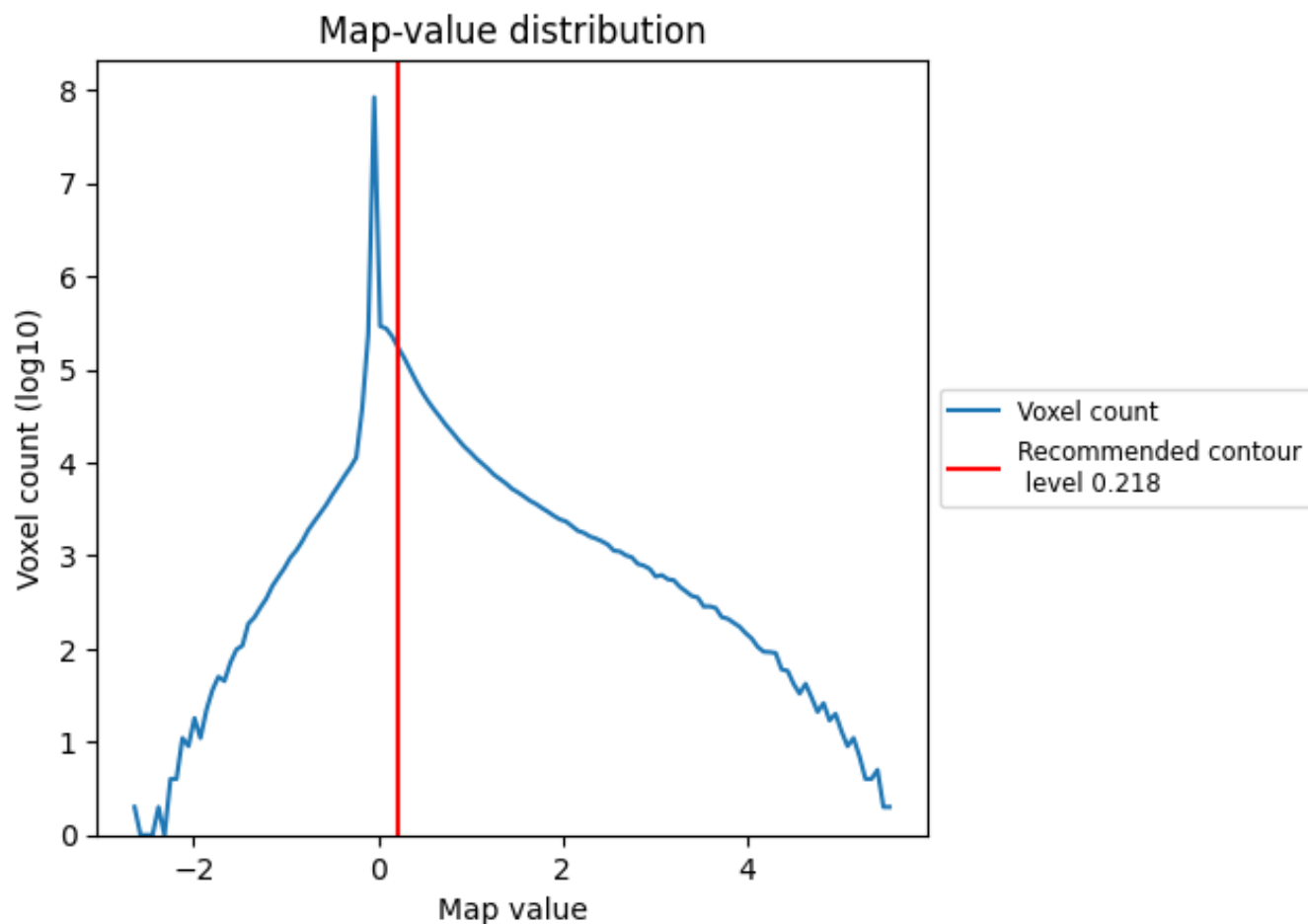
6.5 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

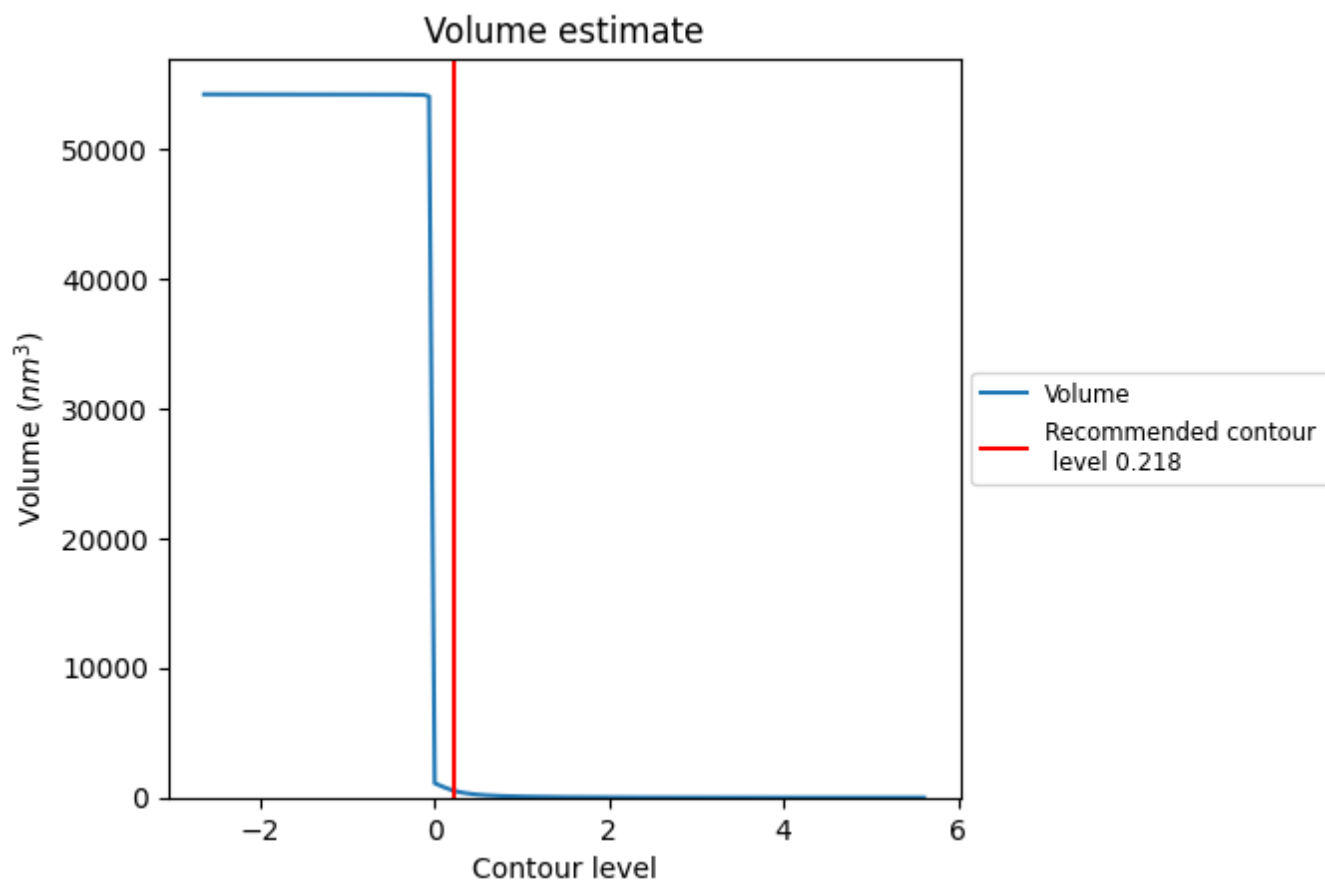
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

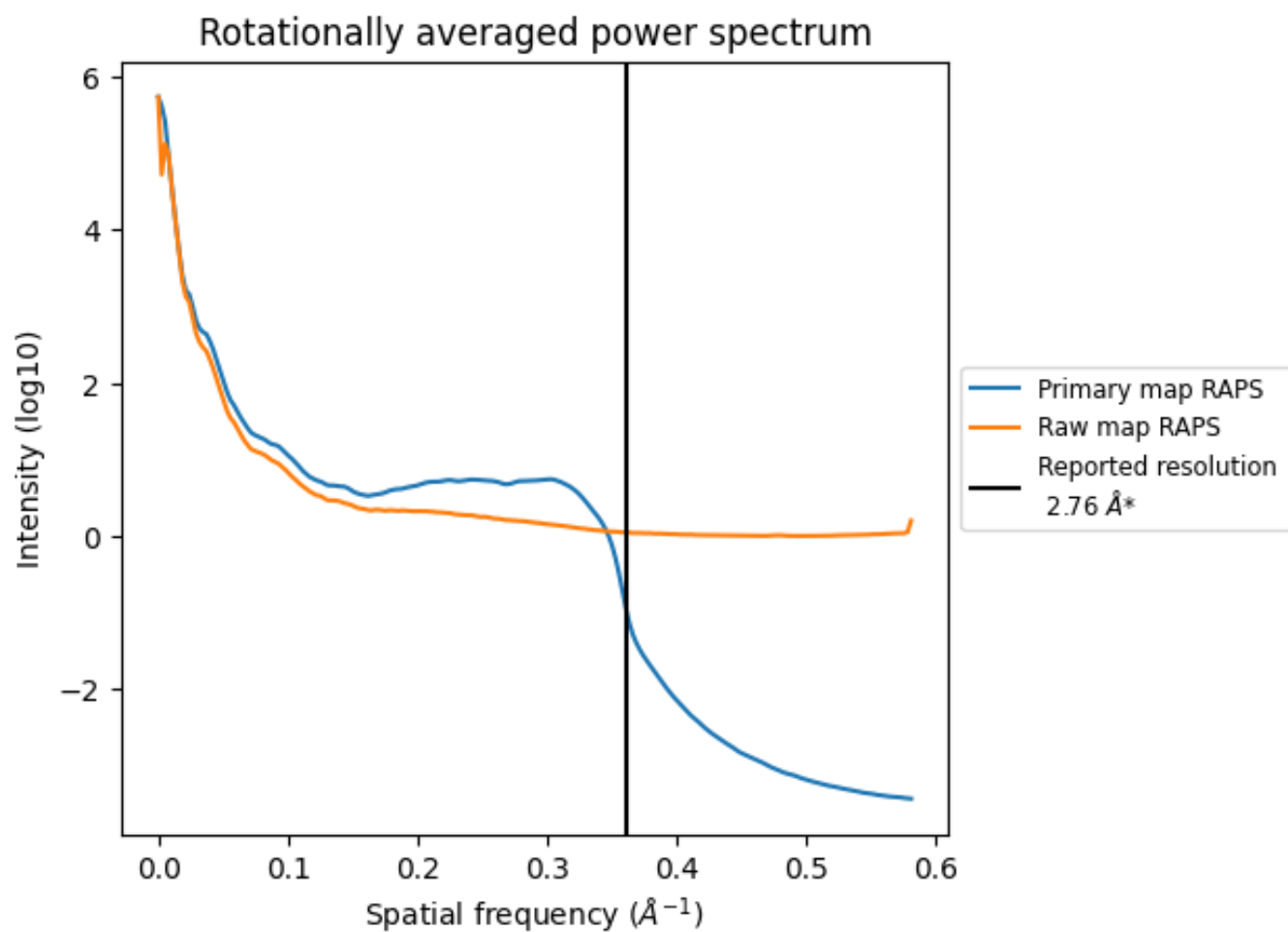
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 544 nm³; this corresponds to an approximate mass of 491 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [\(i\)](#)

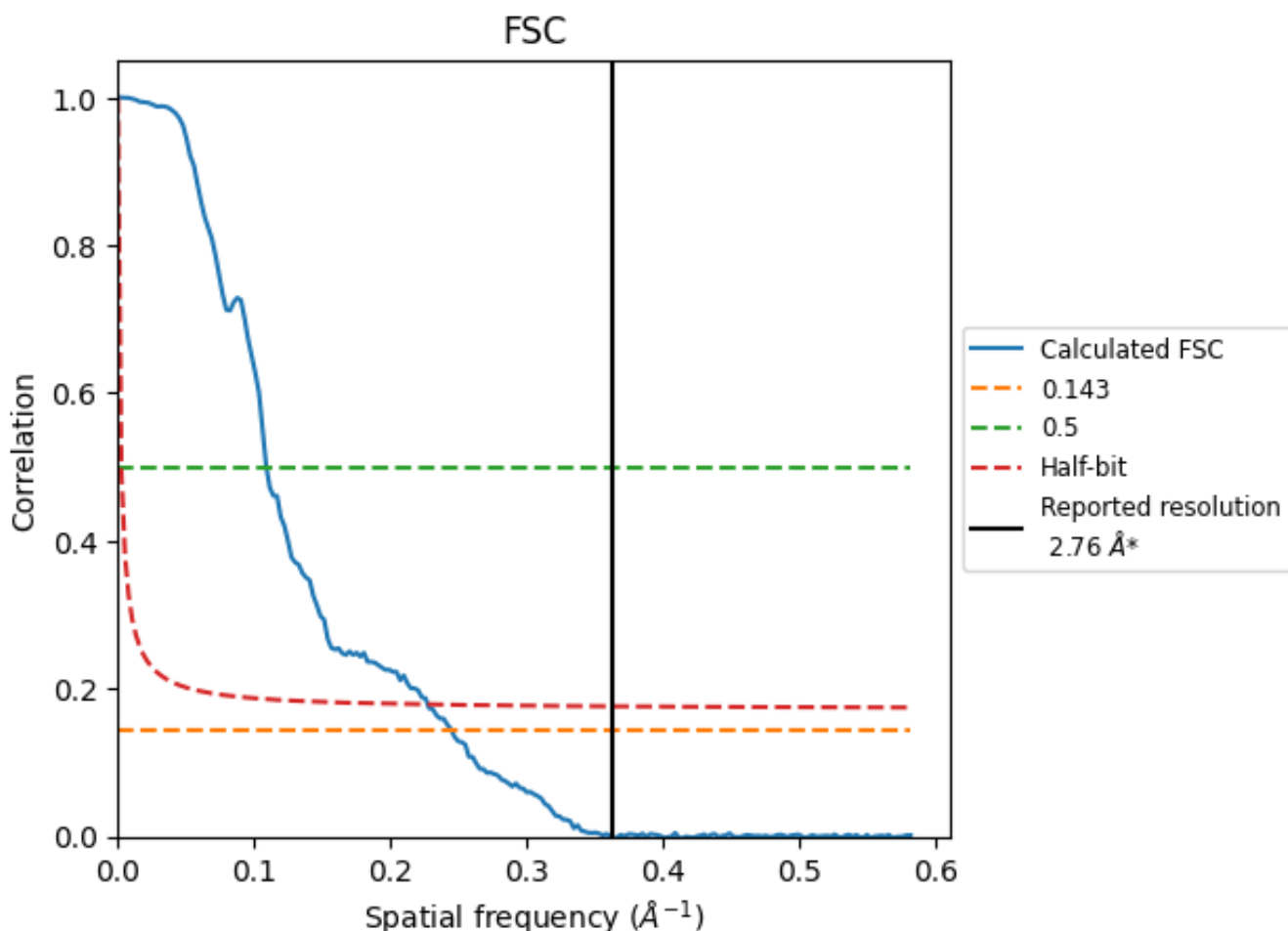


*Reported resolution corresponds to spatial frequency of 0.362 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.362 Å⁻¹

8.2 Resolution estimates [i](#)

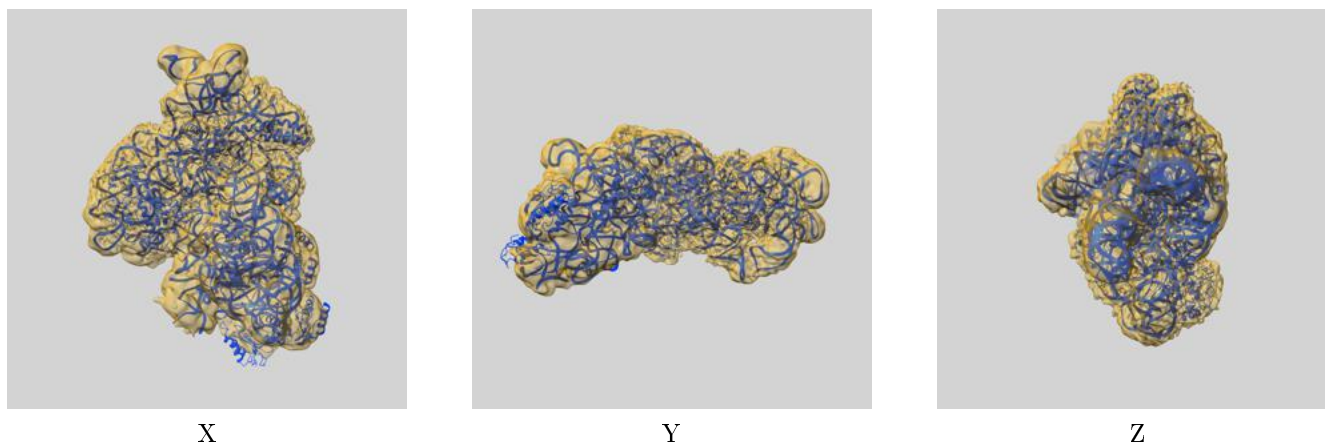
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.76 | - | - |
| Author-provided FSC curve | - | - | - |
| Calculated* | 4.08 | 9.17 | 4.40 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.08 differs from the reported value 2.76 by more than 10 %

9 Map-model fit [i](#)

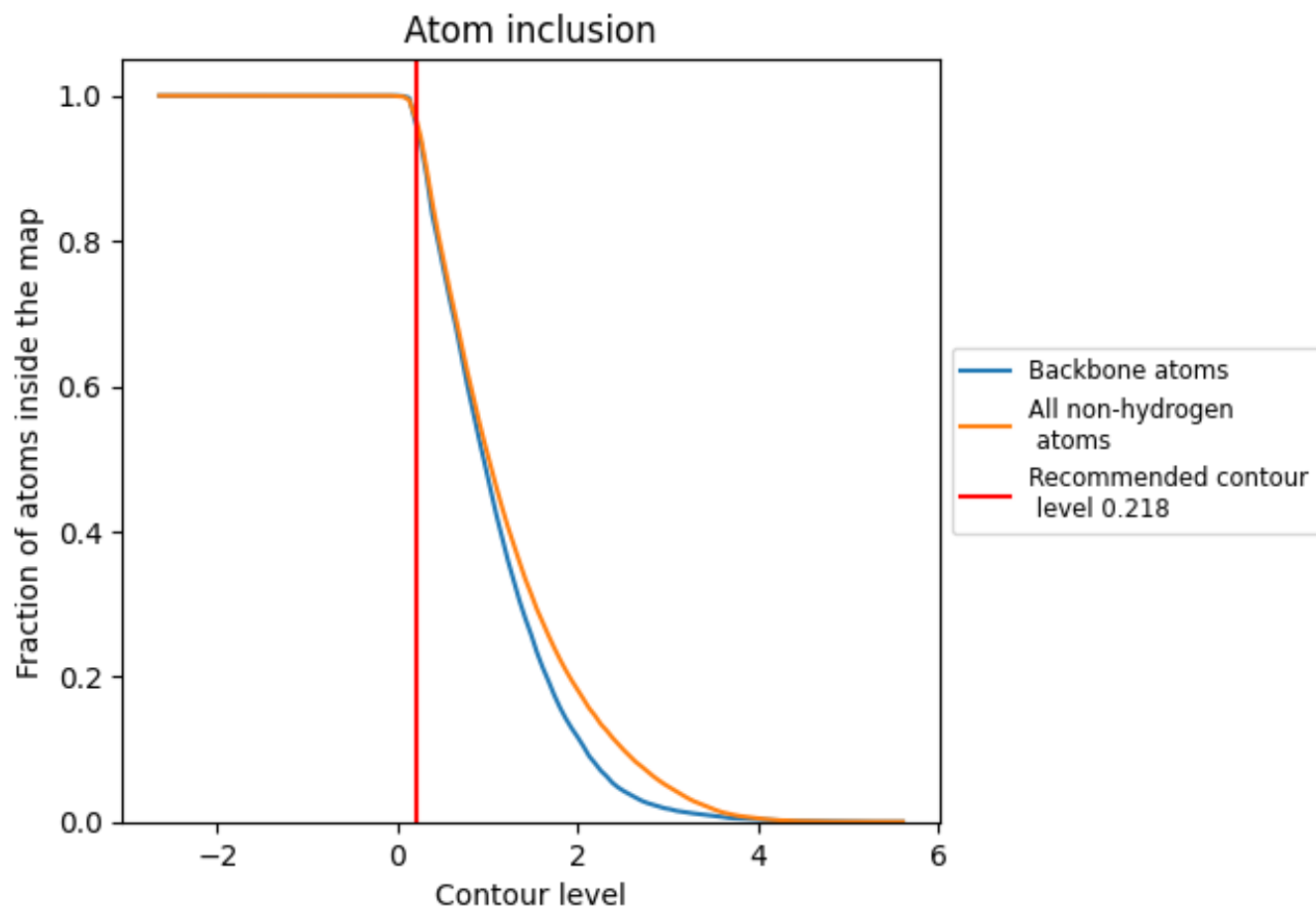
This section contains information regarding the fit between EMDB map EMD-12916 and PDB model 7OI0. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.218 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.